```
=> d his

     (FILE 'HOME' ENTERED AT 11:19:30 ON 06 MAY 2001)

     FILE 'REGISTRY' ENTERED AT 11:19:42 ON 06 MAY 2001
L1                STRUCTURE UPLOADED
L2             50 S L1
L3                STRUCTURE UPLOADED
L4             50 S L3
L5                STRUCTURE UPLOADED
L6             35 S L5
L7            428 S L5 FULL

     FILE 'CAPLUS, USPATFULL' ENTERED AT 11:23:09 ON 06 MAY 2001
L8            452 S L7
L9             10 S L8 AND ((CA OR CALCIUM) (P) CHANNEL)
L10            10 DUP REM L9 (0 DUPLICATES REMOVED)

     FILE 'REGISTRY' ENTERED AT 11:28:55 ON 06 MAY 2001
L11             2 S MIBEFRADIL
L12            87 S L8 AND ?BIS

     FILE 'CAPLUS, USPATFULL' ENTERED AT 11:36:48 ON 06 MAY 2001
L13            98 S L8 AND BIS?
L14             4 S L8 AND DIMER

     FILE 'STNGUIDE' ENTERED AT 11:41:50 ON 06 MAY 2001

     FILE 'REGISTRY' ENTERED AT 11:45:18 ON 06 MAY 2001
L15               STRUCTURE UPLOADED
L16             3 S L15
L17            31 S L15 FULL

     FILE 'CAPLUS, USPATFULL, MEDLINE' ENTERED AT 11:46:19 ON 06 MAY 2001
L18            11 S L17

     FILE 'REGISTRY' ENTERED AT 11:47:58 ON 06 MAY 2001
L19             3 S CLENTIAZEM

     FILE 'CAPLUS' ENTERED AT 11:48:39 ON 06 MAY 2001

     FILE 'REGISTRY' ENTERED AT 11:48:42 ON 06 MAY 2001

     FILE 'REGISTRY' ENTERED AT 11:49:12 ON 06 MAY 2001
L20            21 S DILTIAZEM

=> d l5
L5 HAS NO ANSWERS
L5                STR
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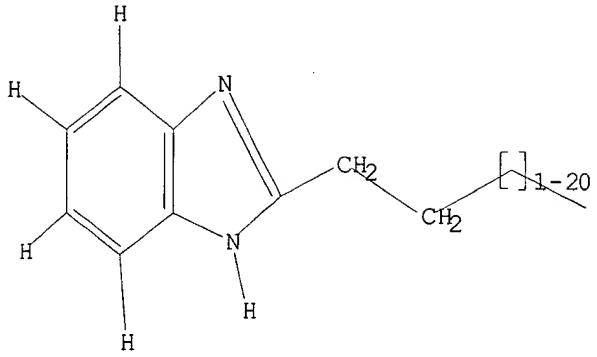
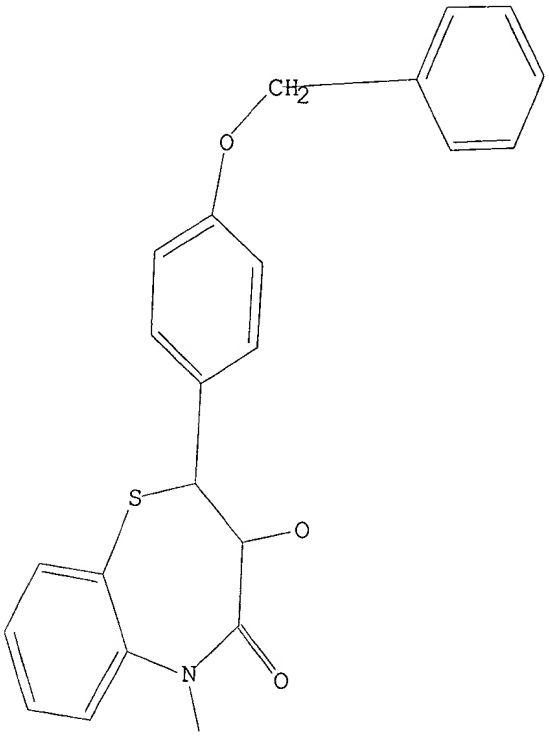


Structure attributes must be viewed using STN Express query preparation.

=> d l15
L15 HAS NO ANSWERS
L15 STR



Structure attributes must be viewed using STN Express query preparation.

=>

14 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1995:776400 CAPLUS
DOCUMENT NUMBER: 123:245168
TITLE: Synthesis, Characterization, Spectroscopy, and Magnetism of Dinuclear Azido- and Alkoxo-Bridged Copper(II) Complexes of Bis(2-benzimidazolyl)alkanes. X-ray Structures of [Cu2(tbz)2(CH3O)2](ClO4)2(CH3OH)2, [Cu2(tbz)2(NO3)(CH3O)2](NO3)(CH3OH)2, and [Cu(tbz)(N3)2]2(CH3OH)2 (tbz = Bis(2-benzimidazolyl)propane)
AUTHOR(S): Van Albada, Gerard A.; Lakin, Miles T.; Veldman, Nora; Spek, Anthony L.; Reedijk, Jan
CORPORATE SOURCE: Leiden Institute of Chemistry, Leiden University, Leiden, 2300 RA, Neth.
SOURCE: Inorg. Chem. (1995), 34(19), 4910-17
CODEN: INOCAJ; ISSN: 0020-1669
DOCUMENT TYPE: Journal
LANGUAGE: English

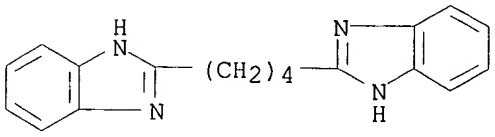
AB A group of new compds. Cu(L)(sol-)(A-)(Hsol), where A = ClO4-, CF3SO3-, BF4-, and NO3-, L = bis(2-benzimidazolyl)propane (abbreviated as tbz) and bis(2-benzimidazolyl)butane (abbreviated as qbz), and Hsol = MeOH and EtOH, and [Cu(tbz)(N3-)(Hsol)] was prepd. and characterized structurally, magnetically, and spectroscopically. Three representative compds. [Cu2(tbz)2(MeO)2](ClO4)2(MeOH)2 (1), [Cu2(tbz)2(NO3)(MeO)2](NO3)(MeOH)2 (5), and [Cu(tbz)(N3)2]2(MeOH)2 (13) were characterized structurally with x-ray diffraction. Crystal data for 1: monoclinic, space group P21/c with a 9.6863(10), b 12.9445(10), c 19.394(2) .ANG., .beta. 113.259(10).degree., and Z = 2. Crystal data for 5: monoclinic, space group P21 with a 9.5497(6), b 12.5073(7), c 17.5920(12) .ANG., .beta. 90.996(6).degree., and Z = 2. Crystal data for 13: orthorhombic, space group Pbca with a 11.3325(7), b 18.7096(16), c 19.2011(16) .ANG., and Z = 4. The structure refinement converged to wR2 = 0.1381, R1 = 0.0534 for 1, wR2 = 0.0674, R1 = 0.0271 for 5, and wR2 = 0.1119, R1 = 0.0701 for 13. The structures 1 and 5 consist of dinuclear units with bridging methoxo groups and one ligand linked to each Cu via the N, providing square planar CuN2O2 chromophores. Structure 5 consists of a dinuclear unit in which one of the Cu atoms is linked to a nitrate O, to yield a unit with two different Cu environments, one square planar and the other square pyramidal. Structure 13 consists also of dinuclear units with the two Cu atoms bridged by .mu.-(1,1)-azido groups. Also each Cu is surrounded by two nitrogens of the ligand and a N of a nonbridging end-on .mu.-(1,1)-azido moiety resulting in a distorted square pyramidal geometry. The Cu-Cu distances (.ANG.) within the dinuclear units are as follows: 1, 2.9827(6); 5, 3.0072(4); 13, 3.2422(9). The Cu-O-Cu bridging angles (deg) are as follows: 1, 102.89(14); 5, 103.97(9), 103.06(9).degree.. The Cu-N-Cu bridging angle for 13 is 104.66(17).degree.. Far-IR spectroscopy shows bands which are characteristic for the bridging Cu2O2N4 chromophore; Cu-O vibrations are found at .apprx.457 and 330 cm-1 for the ethoxo-bridged compds. and at .apprx.390 and 232 cm-1 for the methoxo-bridged compds. The magnetic susceptibility measurements of the alkoxo-bridged compds. display a diamagnetic behavior below room temp. with an estd. exchange parameter 2J of <-600 cm-1. These dinuclear species are EPR silent, and only a weak signal of monomeric impurities is obsd. The .mu.-(1,1)-azido-bridged **dimer** shows a ferromagnetic behavior with a calcd. J value of +23

cm-1 and a weak, very broad isotropic EPR signal at g = 2.14.

IT **4746-56-9**, 1,4-Bis(2-benzimidazolyl)butane
RL: RCT (Reactant)
(for prepn. of copper dinuclear alkoxo-bridged complexes)

RN 4746-56-9 CAPLUS

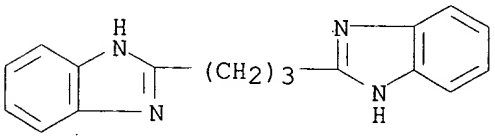
CN 1H-Benzimidazole, 2,2'-(1,4-butanediyl)bis- (9CI) (CA INDEX NAME)



IT **7147-66-2**, 1,3-Bis(2-benzimidazolyl)propane
RL: RCT (Reactant)
(for prepn. of copper dinuclear azido-, alkoxo- and alkoxo/nitrato-bridged complexes)

RN 7147-66-2 CAPLUS

CN 1H-Benzimidazole, 2,2'-(1,3-propanediyl)bis- (9CI) (CA INDEX NAME)



=>

Medted species

31 ANSWERS

```
=> s l15 full
FULL SEARCH INITIATED 11:46:09 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -     389 TO ITERATE

100.0% PROCESSED     389 ITERATIONS
SEARCH TIME: 00.00.01

L17           31 SEA SSS FUL L15

=> file caplu uspatful medlin
COST IN U.S. DOLLARS                                  SINCE FILE      TOTAL
                                                         ENTRY    SESSION
FULL ESTIMATED COST                                     133.87     368.41

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)            SINCE FILE      TOTAL
                                                         ENTRY    SESSION
CA SUBSCRIBER PRICE                                       0.00      -1.18

FILE 'CAPLUS' ENTERED AT 11:46:19 ON 06 MAY 2001
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2001 AMERICAN CHEMICAL SOCIETY (ACS)

FILE 'USPATFULL' ENTERED AT 11:46:19 ON 06 MAY 2001
CA INDEXING COPYRIGHT (C) 2001 AMERICAN CHEMICAL SOCIETY (ACS)

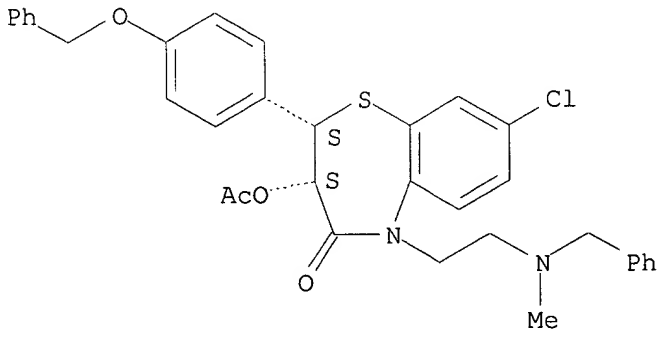
FILE 'MEDLINE' ENTERED AT 11:46:19 ON 06 MAY 2001

=> s l17
L18           11 L17

=> d hitstr 1-
YOU HAVE REQUESTED DATA FROM 11 ANSWERS - CONTINUE? Y/(N):y

L18  ANSWER 1 OF 11  CAPLUS  COPYRIGHT 2001 ACS
IT   112525-50-5P 112525-51-6P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (prepn. of, as intermediate for clentiazem metabolite)
RN   112525-50-5  CAPLUS
CN   1,5-Benzothiazepin-4(5H)-one, 3-(acetyloxy)-8-chloro-2,3-dihydro-5-[2-
     [methyl(phenylmethyl)amino]ethyl]-2-[4-(phenylmethoxy)phenyl]-, (2S-cis)-
     (9CI)  (CA INDEX NAME)

Absolute stereochemistry.
```

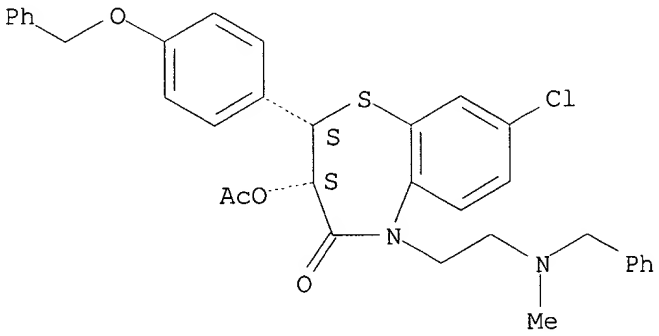


RN 112525-51-6 CAPLUS
CN 1,5-Benzothiazepin-4(5H)-one, 3-(acetyloxy)-8-chloro-2,3-dihydro-5-[2-[methyl(phenylmethyl)amino]ethyl]-2-[4-(phenylmethoxy)phenyl]-, (2S-cis)-, ethanedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

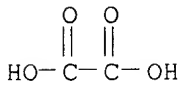
CRN 112525-50-5
CMF C34 H33 Cl N2 O4 S
CDES *

Absolute stereochemistry.



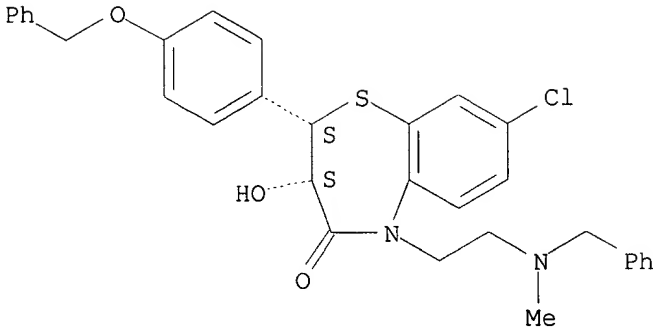
CM 2

CRN 144-62-7
CMF C2 H2 O4



IT **112525-30-1P 112525-31-2P 112525-45-8P 112525-46-9P 112525-54-9P 112544-49-7P 156415-90-6P 156415-91-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, clentiazem metabolite)
RN 112525-30-1 CAPLUS
CN 1,5-Benzothiazepin-4(5H)-one, 8-chloro-2,3-dihydro-3-hydroxy-5-[2-[methyl(phenylmethyl)amino]ethyl]-2-[4-(phenylmethoxy)phenyl]-, (2S-cis)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

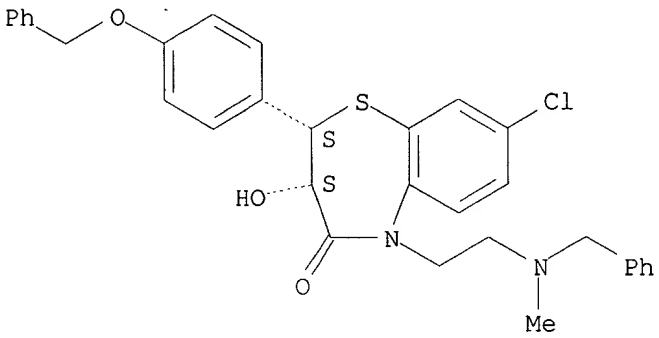


RN 112525-31-2 CAPLUS
CN 1,5-Benzothiazepin-4(5H)-one, 8-chloro-2,3-dihydro-3-hydroxy-5-[2-[methyl(phenylmethyl)amino]ethyl]-2-[4-(phenylmethoxy)phenyl]-, (2S-cis)-, ethanedioate (1:1) (salt) (9CI) (CA INDEX NAME)

CM 1

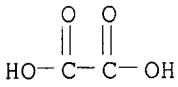
CRN 112525-30-1
CMF C32 H31 Cl N2 O3 S
CDES *

Absolute stereochemistry.



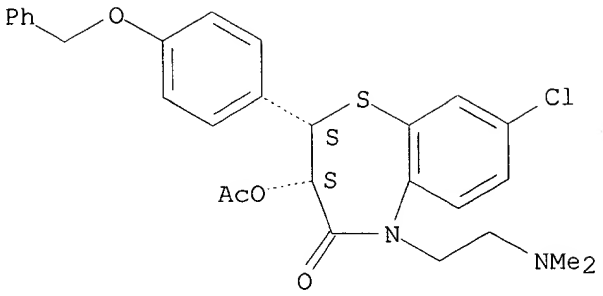
CM 2

CRN 144-62-7
CMF C2 H2 O4



RN 112525-45-8 CAPLUS
CN 1,5-Benzothiazepin-4(5H)-one, 3-(acetyloxy)-8-chloro-5-[2-(dimethylamino)ethyl]-2,3-dihydro-2-[4-(phenylmethoxy)phenyl]-, (2S-cis)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

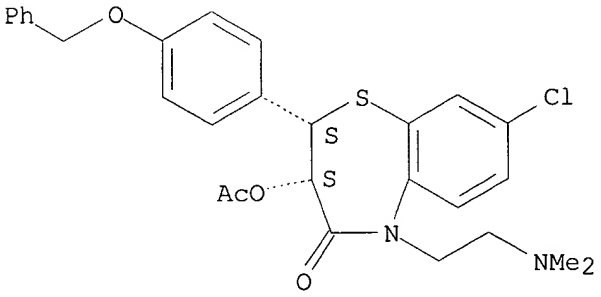


RN 112525-46-9 CAPLUS
CN 1,5-Benzothiazepin-4(5H)-one, 3-(acetyloxy)-8-chloro-5-[2-(dimethylamino)ethyl]-2,3-dihydro-2-[4-(phenylmethoxy)phenyl]-, (2S-cis)-, ethanedioate (2:1) (9CI) (CA INDEX NAME)

CM 1

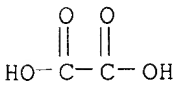
CRN 112525-45-8
CMF C28 H29 Cl N2 O4 S
CDES *

Absolute stereochemistry.



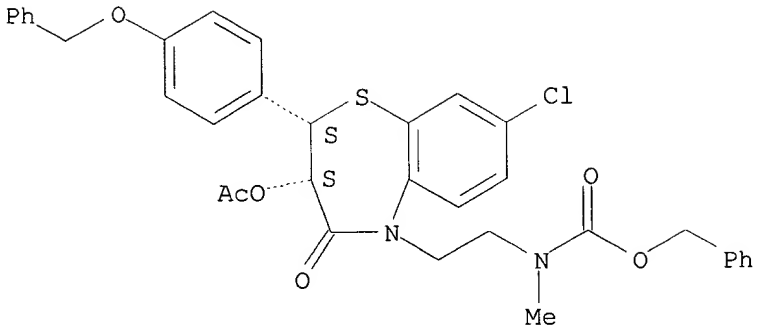
CM 2

CRN 144-62-7
CMF C2 H2 O4



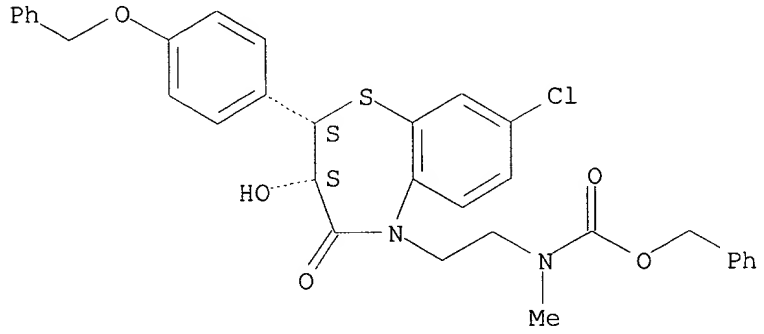
RN 112525-54-9 CAPLUS
CN Carbamic acid, [2-[3-(acetyloxy)-8-chloro-3,4-dihydro-4-oxo-2-[4-(phenylmethoxy)phenyl]-1,5-benzothiazepin-5(2H)-yl]ethyl]methyl-, phenylmethyl ester, (2S-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



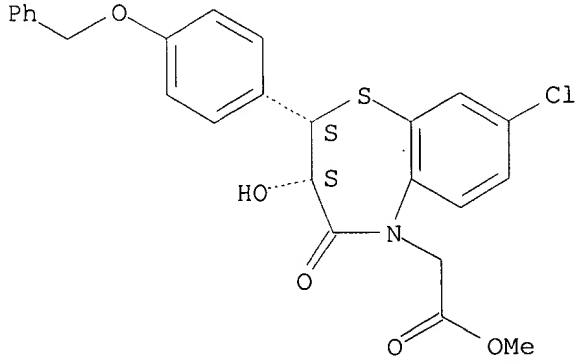
RN 112544-49-7 CAPLUS
CN Carbamic acid, [2-[8-chloro-3,4-dihydro-3-hydroxy-4-oxo-2-[4-(phenylmethoxy)phenyl]-1,5-benzothiazepin-5(2H)-yl]ethyl]methyl-, phenylmethyl ester, (2S-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 156415-90-6 CAPLUS
CN 1,5-Benzothiazepine-5(2H)-acetic acid, 8-chloro-3,4-dihydro-3-hydroxy-4-oxo-2-[4-(phenylmethoxy)phenyl]-, methyl ester, (2S-cis)- (9CI) (CA INDEX NAME)

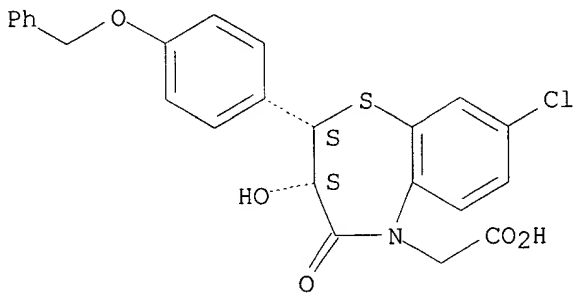
Absolute stereochemistry.



RN 156415-91-7 CAPLUS
CN 1,5-Benzothiazepine-5(2H)-acetic acid, 8-chloro-3,4-dihydro-3-hydroxy-4-

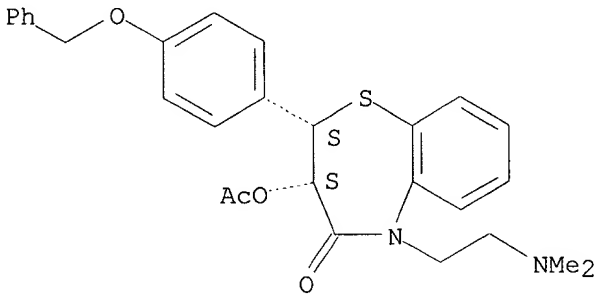
oxo-2-[4-(phenylmethoxy)phenyl]-, (2S-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



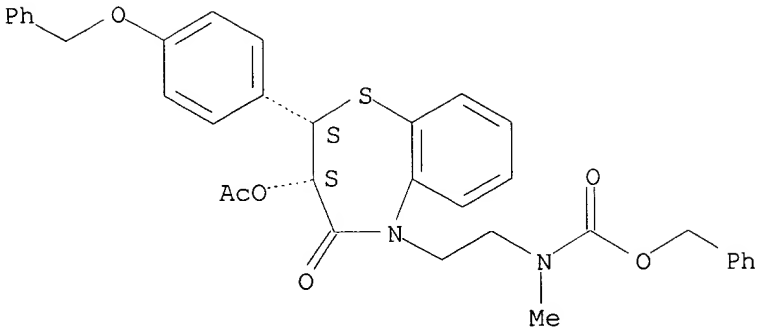
L18 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2001 ACS
IT **84903-76-4P 142843-03-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and deprotection of)
RN 84903-76-4 CAPLUS
CN 1,5-Benzothiazepin-4(5H)-one,
3-(acetyloxy)-5-[2-(dimethylamino)ethyl]-2,3-
dihydro-2-[4-(phenylmethoxy)phenyl]-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



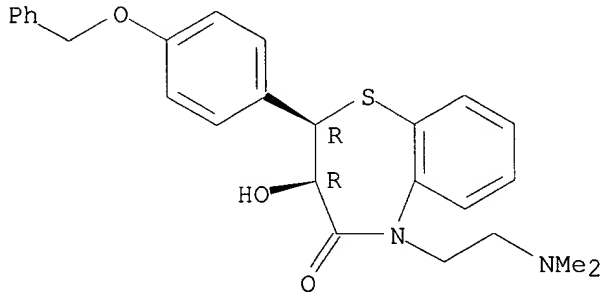
RN 142843-03-6 CAPLUS
CN Carbamic acid, [2-[3-(acetyloxy)-3,4-dihydro-4-oxo-2-[4-
(phenylmethoxy)phenyl]-1,5-benzothiazepin-5(2H)-yl]ethyl]methyl-,
phenylmethyl ester, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



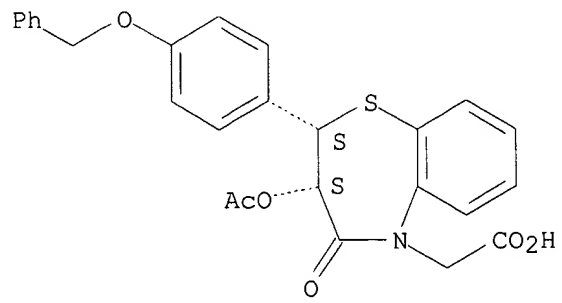
IT **142843-01-4P 142843-02-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn., acetylation, and deprotection of)
RN 142843-01-4 CAPLUS
RN 142843-02-5 CAPLUS
CN 1,5-Benzothiazepin-4(5H)-one, 5-[2-(dimethylamino)ethyl]-2,3-dihydro-3-hydroxy-2-[4-(phenylmethoxy)phenyl]-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



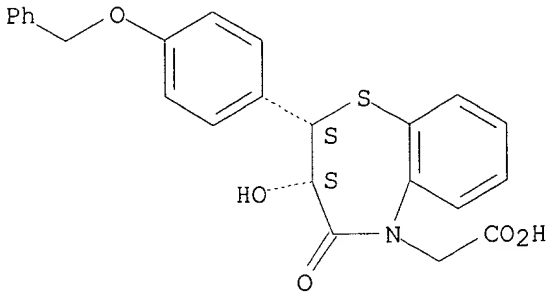
L18 ANSWER 3 OF 11 CAPLUS COPYRIGHT 2001 ACS
IT **115973-34-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and debenzylation of)
RN 115973-34-7 CAPLUS
CN 1,5-Benzothiazepine-5(2H)-acetic acid, 3-(acetyloxy)-3,4-dihydro-4-oxo-2-[4-(phenylmethoxy)phenyl]-, (2S-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



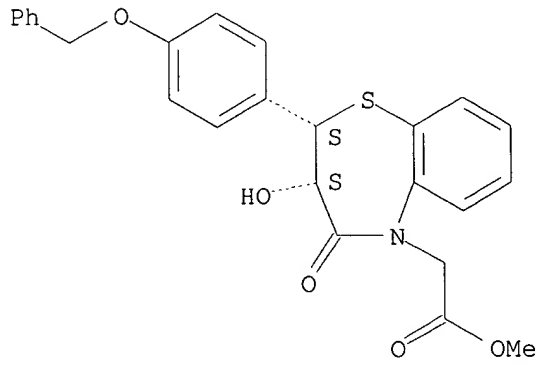
IT **115973-33-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and debenzylation or acetylation of)
RN 115973-33-6 CAPLUS
CN 1,5-Benzothiazepine-5(2H)-acetic acid, 3,4-dihydro-3-hydroxy-4-oxo-2-[4-(phenylmethoxy)phenyl]-, (2S-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **115992-92-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and hydrolysis of)
RN 115992-92-2 CAPLUS
CN 1,5-Benzothiazepine-5(2H)-acetic acid, 3,4-dihydro-3-hydroxy-4-oxo-2-[4-(phenylmethoxy)phenyl]-, methyl ester, (2S-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



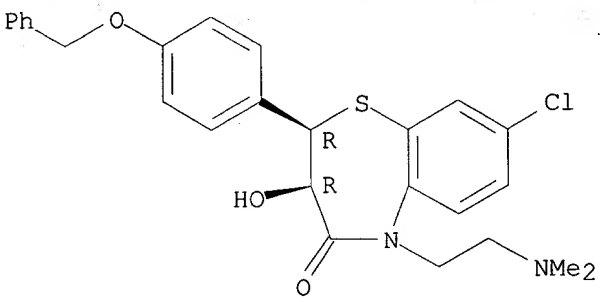
L18 ANSWER 4 OF 11 CAPLUS COPYRIGHT 2001 ACS
IT **112525-38-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and acetylation of)
RN 112525-38-9 CAPLUS
CN 1,5-Benzothiazepin-4(5H)-one, 8-chloro-5-[2-(dimethylamino)ethyl]-2,3-dihydro-3-hydroxy-2-[4-(phenylmethoxy)phenyl]-, cis-(+)-, ethanedioate (1:1) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 112525-37-8
CMF C26 H27 Cl N2 O3 S

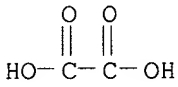
CDES 2:CIS3:(+)

Rotation (+). Absolute stereochemistry unknown.



CM 2

CRN 144-62-7
CMF C2 H2 O4

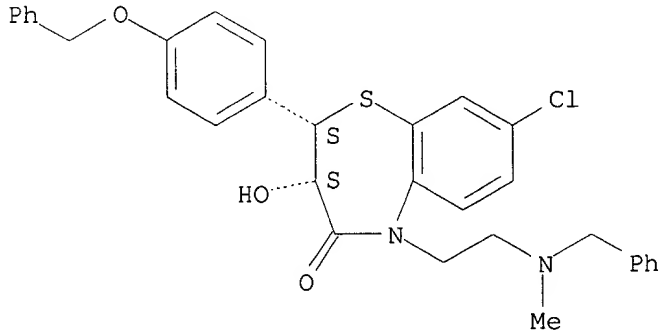


IT **112525-31-2P 112525-51-6P 112525-53-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and debenzylation and N-acylation of)
RN 112525-31-2 CAPLUS
CN 1,5-Benzothiazepin-4(5H)-one, 8-chloro-2,3-dihydro-3-hydroxy-5-[2-[methyl(phenylmethyl)amino]ethyl]-2-[4-(phenylmethoxy)phenyl]-, (2S-cis)-,
ethanedioate (1:1) (salt) (9CI) (CA INDEX NAME)

CM 1

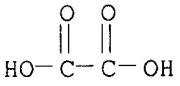
CRN 112525-30-1
CMF C32 H31 Cl N2 O3 S
CDES *

Absolute stereochemistry.



CM 2

CRN 144-62-7
CMF C2 H2 O4

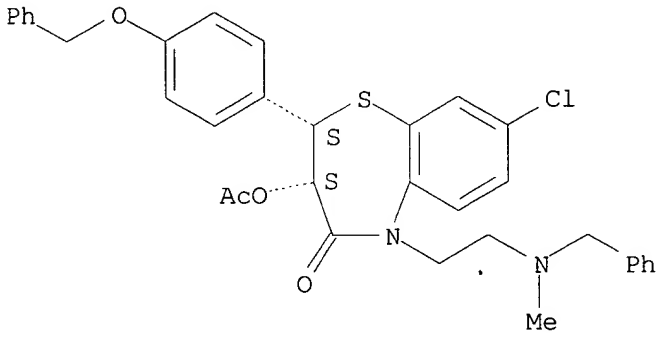


RN 112525-51-6 CAPLUS
CN 1,5-Benzothiazepin-4(5H)-one, 3-(acetyloxy)-8-chloro-2,3-dihydro-5-[2-[methyl(phenylmethyl)amino]ethyl]-2-[4-(phenylmethoxy)phenyl]-, (2S-cis)-, ethanedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

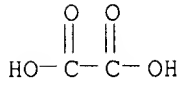
CRN 112525-50-5
CMF C34 H33 Cl N2 O4 S
CDES *

Absolute stereochemistry.



CM 2

CRN 144-62-7
CMF C2 H2 O4

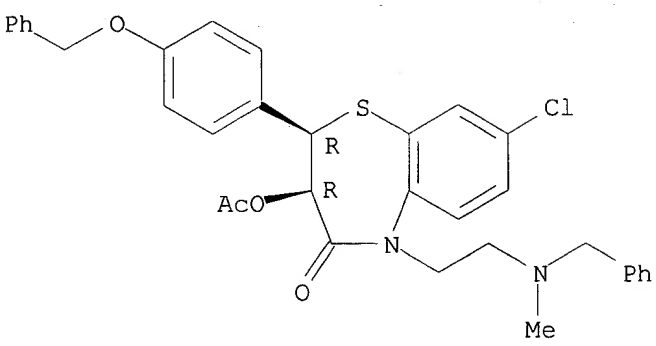


RN 112525-53-8 CAPLUS
CN 1,5-Benzothiazepin-4(5H)-one, 3-(acetyloxy)-8-chloro-2,3-dihydro-5-[2-[methyl(phenylmethyl)amino]ethyl]-2-[4-(phenylmethoxy)phenyl]-, (2R-cis)-, ethanedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

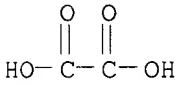
CRN 112525-52-7
CMF C34 H33 Cl N2 O4 S
CDES *

Absolute stereochemistry.



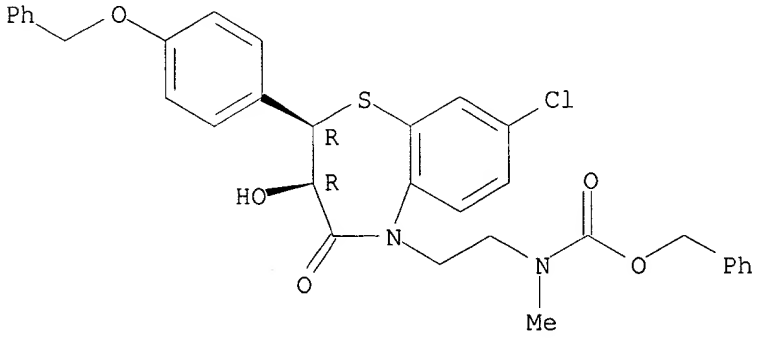
CM 2

CRN 144-62-7
CMF C2 H2 O4



IT **112525-34-5P 112525-46-9P 112525-54-9P**
112544-49-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and deprotection of)
RN 112525-34-5 CAPLUS
CN Carbamic acid, [2-[8-chloro-3,4-dihydro-3-hydroxy-4-oxo-2-[4-(phenylmethoxy)phenyl]-1,5-benzothiazepin-5(2H)-yl]ethyl]methyl-, phenylmethyl ester, (2R-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



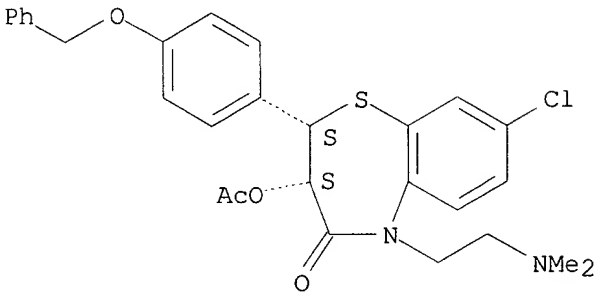
RN 112525-46-9 CAPLUS
CN 1,5-Benzothiazepin-4(5H)-one, 3-(acetyloxy)-8-chloro-5-[2-(dimethylamino)ethyl]-2,3-dihydro-2-[4-(phenylmethoxy)phenyl]-, (2S-cis)-,

ethanedioate (2:1) (9CI) (CA INDEX NAME)

CM 1

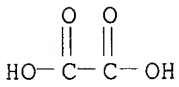
CRN 112525-45-8
CMF C28 H29 Cl N2 O4 S
CDES *

Absolute stereochemistry.



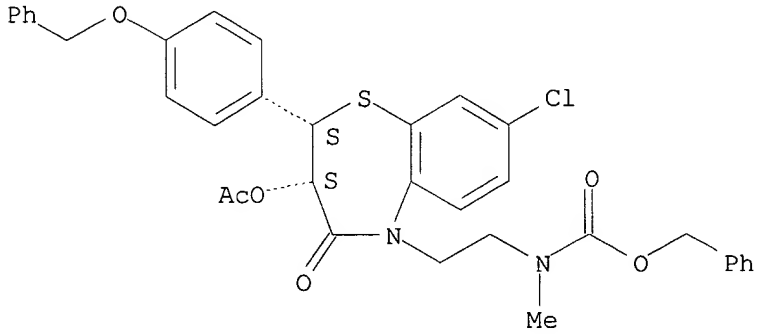
CM 2

CRN 144-62-7
CMF C2 H2 O4



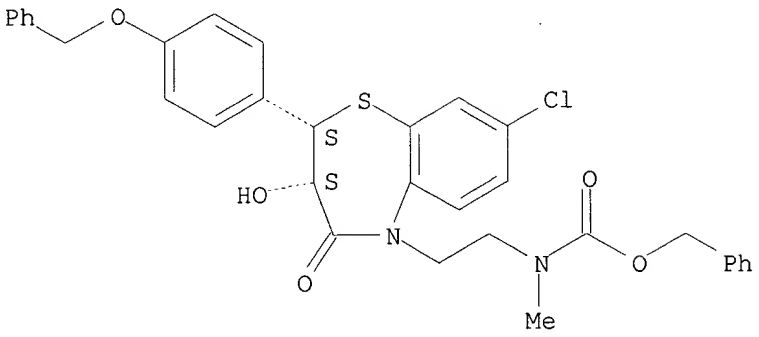
RN 112525-54-9 CAPLUS
CN Carbamic acid, [2-[3-(acetyloxy)-8-chloro-3,4-dihydro-4-oxo-2-[4-(phenylmethoxy)phenyl]-1,5-benzothiazepin-5(2H)-yl]ethyl]methyl-, phenylmethyl ester, (2S-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 112544-49-7 CAPLUS
CN Carbamic acid, [2-[8-chloro-3,4-dihydro-3-hydroxy-4-oxo-2-[4-(phenylmethoxy)phenyl]-1,5-benzothiazepin-5(2H)-yl]ethyl]methyl-, phenylmethyl ester, (2S-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

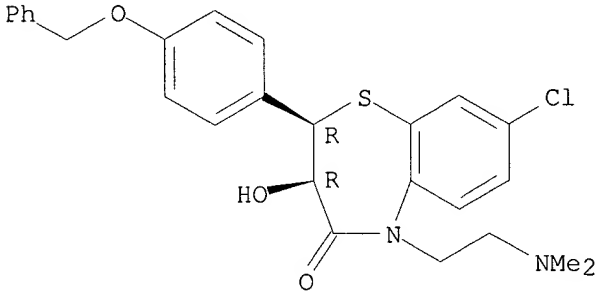


IT **112525-40-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as intermediate for cardiovascular agent)
RN 112525-40-3 CAPLUS
CN 1,5-Benzothiazepin-4(5H)-one, 8-chloro-5-[2-(dimethylamino)ethyl]-2,3-dihydro-3-hydroxy-2-[4-(phenylmethoxy)phenyl]-, cis-(-)-, ethanedioate (1:1) (salt) (9CI) (CA INDEX NAME)

CM 1

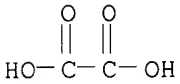
CRN 112525-39-0
CMF C26 H27 Cl N2 O3 S
CDES 2:CIS3:(-)

Rotation (-). Absolute stereochemistry unknown.



CM 2

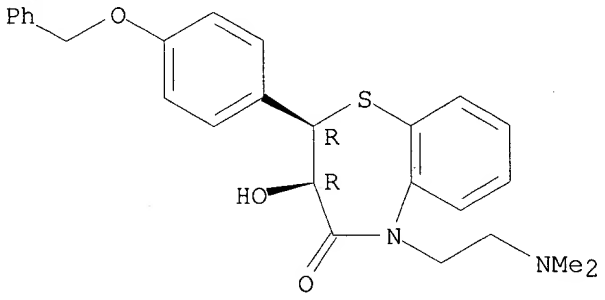
CRN 144-62-7
CMF C2 H2 O4



L18 ANSWER 5 OF 11 CAPLUS COPYRIGHT 2001 ACS

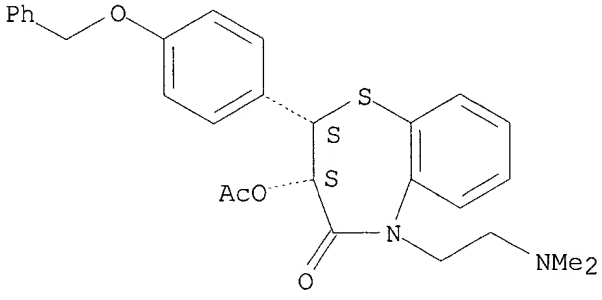
IT **84903-70-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and acetylation of)
RN 84903-70-8 CAPLUS
CN 1,5-Benzothiazepin-4(5H)-one, 5-[2-(dimethylamino)ethyl]-2,3-dihydro-3-hydroxy-2-[4-(phenylmethoxy)phenyl]-, cis-(+)- (9CI) (CA INDEX NAME)

Rotation (+). Absolute stereochemistry unknown.



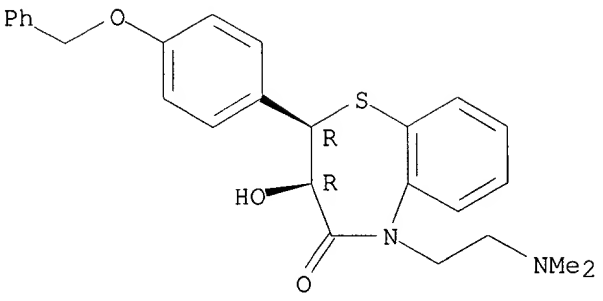
IT **84903-71-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 84903-71-9 CAPLUS
CN 1,5-Benzothiazepin-4(5H)-one,
3-(acetyloxy)-5-[2-(dimethylamino)ethyl]-2,3-dihydro-2-[4-(phenylmethoxy)phenyl]-, cis-(+)- (9CI) (CA INDEX NAME)

Rotation (+). Absolute stereochemistry unknown.



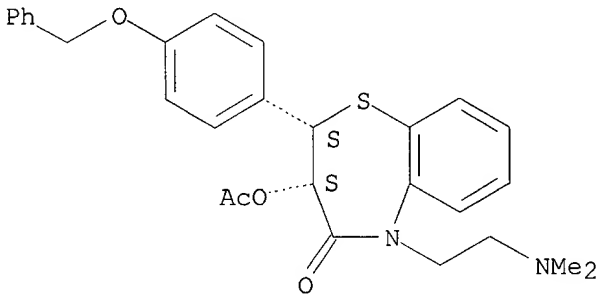
L18 ANSWER 6 OF 11 CAPLUS COPYRIGHT 2001 ACS
IT **84903-70-8P 84903-71-9P 84903-72-0P**
84903-73-1P 84903-74-2P 84903-75-3P
84903-76-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 84903-70-8 CAPLUS
CN 1,5-Benzothiazepin-4(5H)-one, 5-[2-(dimethylamino)ethyl]-2,3-dihydro-3-hydroxy-2-[4-(phenylmethoxy)phenyl]-, cis-(+)- (9CI) (CA INDEX NAME)

Rotation (+). Absolute stereochemistry unknown.



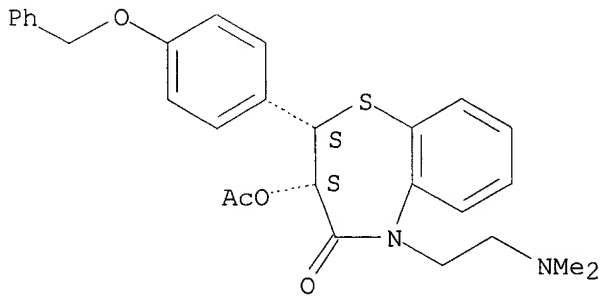
RN 84903-71-9 CAPLUS
CN 1,5-Benzothiazepin-4(5H)-one,
3-(acetyloxy)-5-[2-(dimethylamino)ethyl]-2,3-
dihydro-2-[4-(phenylmethoxy)phenyl]-, cis-(+)- (9CI) (CA INDEX NAME)

Rotation (+). Absolute stereochemistry unknown.



RN 84903-72-0 CAPLUS
CN 1,5-Benzothiazepin-4(5H)-one,
3-(acetyloxy)-5-[2-(dimethylamino)ethyl]-2,3-
dihydro-2-[4-(phenylmethoxy)phenyl]-, monohydrochloride, cis-(+)- (9CI)
(CA INDEX NAME)

Rotation (+). Absolute stereochemistry unknown.

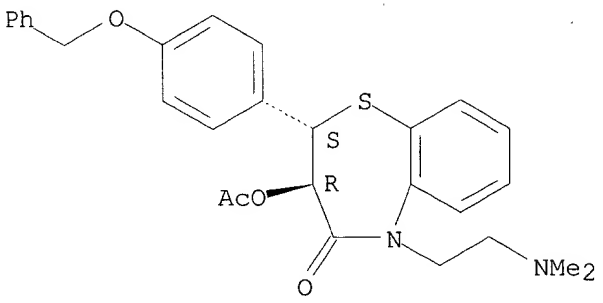


HCl

RN 84903-73-1 CAPLUS
CN 1,5-Benzothiazepin-4(5H)-one,
3-(acetyloxy)-5-[2-(dimethylamino)ethyl]-2,3-

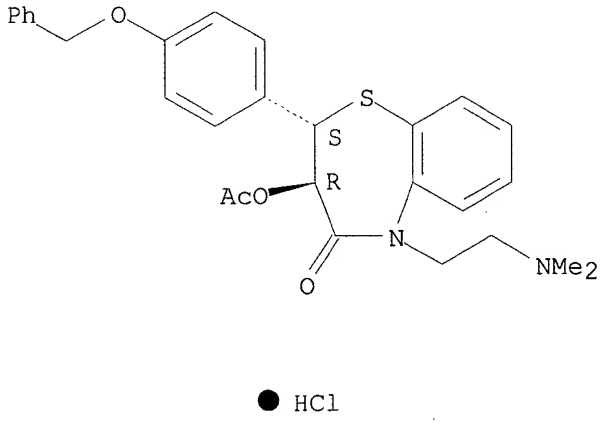
dihydro-2-[4-(phenylmethoxy)phenyl]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



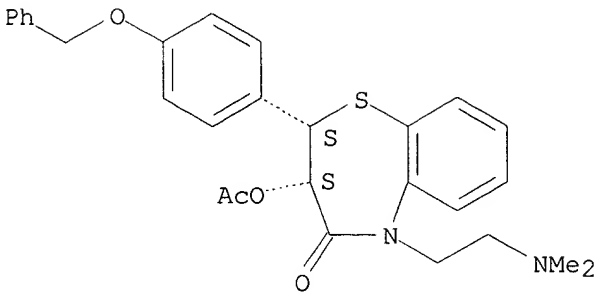
RN 84903-74-2 CAPLUS
CN 1,5-Benzothiazepin-4(5H)-one,
3-(acetyloxy)-5-[2-(dimethylamino)ethyl]-2,3-
dihydro-2-[4-(phenylmethoxy)phenyl]-, monohydrochloride, trans- (9CI)
(CA
INDEX NAME)

Relative stereochemistry.



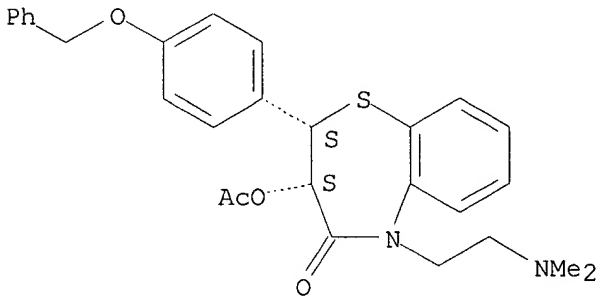
RN 84903-75-3 CAPLUS
CN 1,5-Benzothiazepin-4(5H)-one,
3-(acetyloxy)-5-[2-(dimethylamino)ethyl]-2,3-
dihydro-2-[4-(phenylmethoxy)phenyl]-, cis-(-)- (9CI) (CA INDEX NAME)

Rotation (-). Absolute stereochemistry unknown.



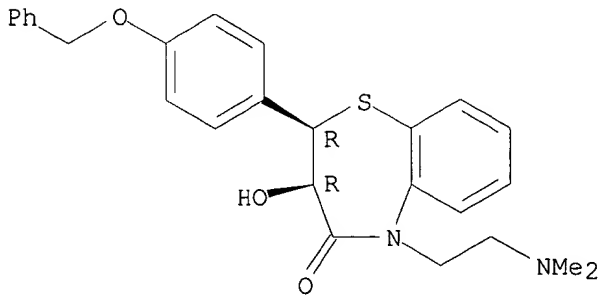
RN 84903-76-4 CAPLUS
CN 1,5-Benzothiazepin-4(5H)-one,
3-(acetyloxy)-5-[2-(dimethylamino)ethyl]-2,3-
dihydro-2-[4-(phenylmethoxy)phenyl]-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L18 ANSWER 7 OF 11 CAPLUS COPYRIGHT 2001 ACS
IT **84903-70-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and acetylation of)
RN 84903-70-8 CAPLUS
CN 1,5-Benzothiazepin-4(5H)-one, 5-[2-(dimethylamino)ethyl]-2,3-dihydro-3-
hydroxy-2-[4-(phenylmethoxy)phenyl]-, cis-(+)- (9CI) (CA INDEX NAME)

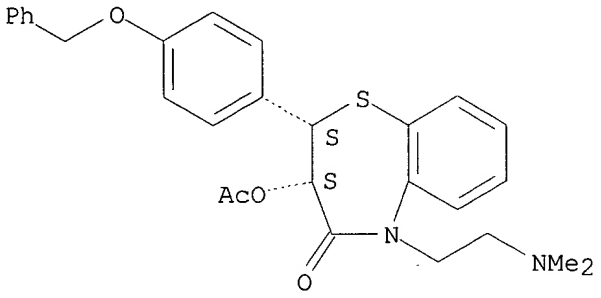
Rotation (+). Absolute stereochemistry unknown.



IT **84903-71-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and debenzylation of)

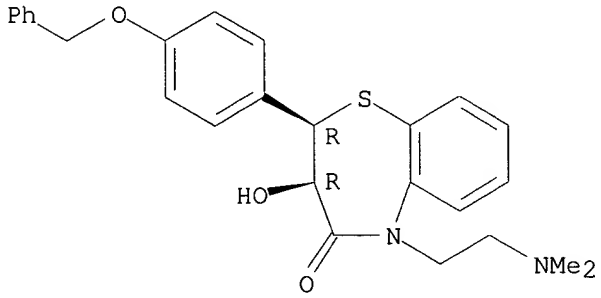
RN 84903-71-9 CAPLUS
CN 1,5-Benzothiazepin-4(5H)-one,
3-(acetyloxy)-5-[2-(dimethylamino)ethyl]-2,3-
dihydro-2-[4-(phenylmethoxy)phenyl]-, cis-(+)- (9CI) (CA INDEX NAME)

Rotation (+). Absolute stereochemistry unknown.



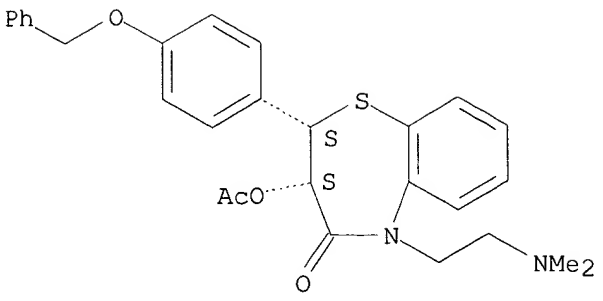
L18 ANSWER 8 OF 11 CAPLUS COPYRIGHT 2001 ACS
IT **84903-70-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and acetylation of)
RN 84903-70-8 CAPLUS
CN 1,5-Benzothiazepin-4(5H)-one, 5-[2-(dimethylamino)ethyl]-2,3-dihydro-3-
hydroxy-2-[4-(phenylmethoxy)phenyl]-, cis-(+)- (9CI) (CA INDEX NAME)

Rotation (+). Absolute stereochemistry unknown.



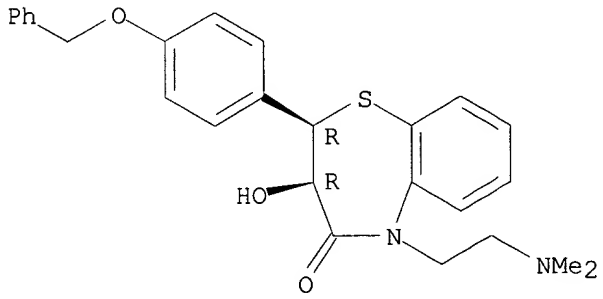
IT **84903-71-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and debenzylation of)
RN 84903-71-9 CAPLUS
CN 1,5-Benzothiazepin-4(5H)-one,
3-(acetyloxy)-5-[2-(dimethylamino)ethyl]-2,3-
dihydro-2-[4-(phenylmethoxy)phenyl]-, cis-(+)- (9CI) (CA INDEX NAME)

Rotation (+). Absolute stereochemistry unknown.



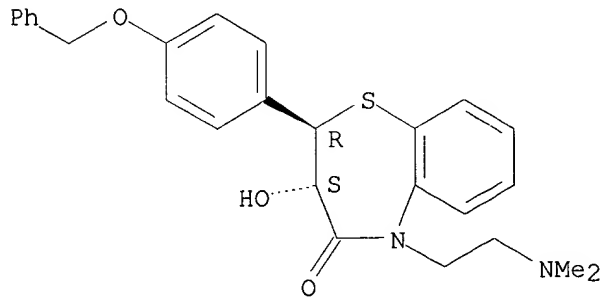
L18 ANSWER 9 OF 11 CAPLUS COPYRIGHT 2001 ACS
IT **84903-70-8P 84914-79-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and acetylation of)
RN 84903-70-8 CAPLUS
CN 1,5-Benzothiazepin-4(5H)-one, 5-[2-(dimethylamino)ethyl]-2,3-dihydro-3-hydroxy-2-[4-(phenylmethoxy)phenyl]-, cis-(+)- (9CI) (CA INDEX NAME)

Rotation (+). Absolute stereochemistry unknown.



RN 84914-79-4 CAPLUS
CN 1,5-Benzothiazepin-4(5H)-one, 5-[2-(dimethylamino)ethyl]-2,3-dihydro-3-hydroxy-2-[4-(phenylmethoxy)phenyl]-, trans- (9CI) (CA INDEX NAME)

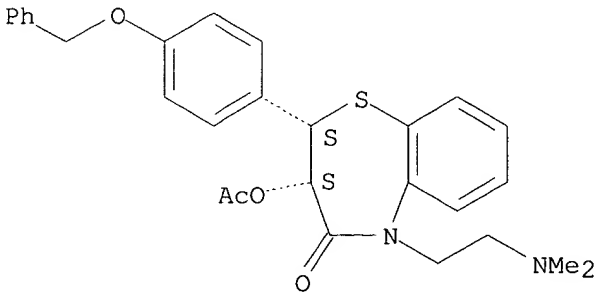
Relative stereochemistry.



IT **84903-71-9P 84903-73-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and debenzylation of)
RN 84903-71-9 CAPLUS

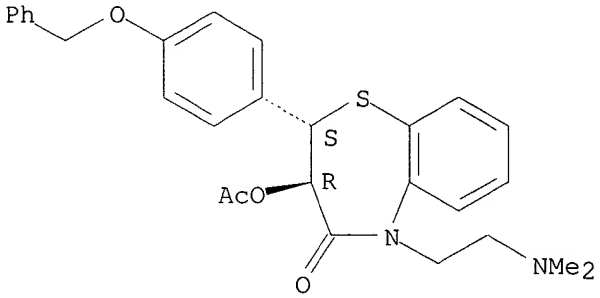
CN 1,5-Benzothiazepin-4(5H)-one,
3-(acetyloxy)-5-[2-(dimethylamino)ethyl]-2,3-
dihydro-2-[4-(phenylmethoxy)phenyl]-, cis-(+)- (9CI) (CA INDEX NAME)

Rotation (+). Absolute stereochemistry unknown.



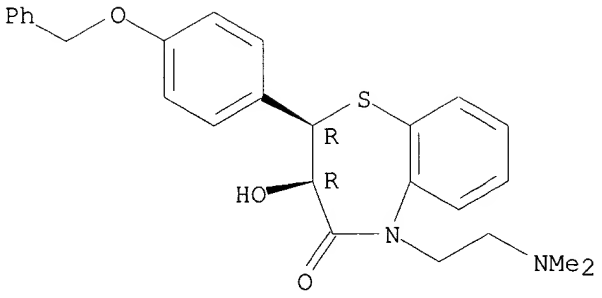
RN 84903-73-1 CAPLUS
CN 1,5-Benzothiazepin-4(5H)-one,
3-(acetyloxy)-5-[2-(dimethylamino)ethyl]-2,3-
dihydro-2-[4-(phenylmethoxy)phenyl]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



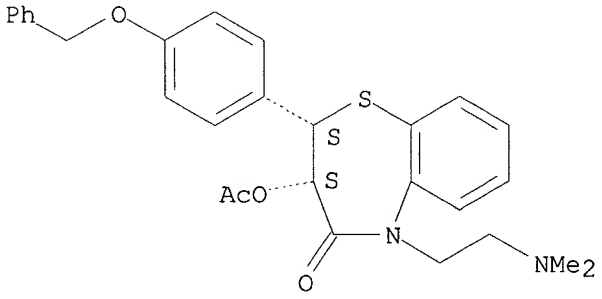
L18 ANSWER 10 OF 11 CAPLUS COPYRIGHT 2001 ACS
IT **84903-70-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and acetylation of)
RN 84903-70-8 CAPLUS
CN 1,5-Benzothiazepin-4(5H)-one, 5-[2-(dimethylamino)ethyl]-2,3-dihydro-3-
hydroxy-2-[4-(phenylmethoxy)phenyl]-, cis-(+)- (9CI) (CA INDEX NAME)

Rotation (+). Absolute stereochemistry unknown.



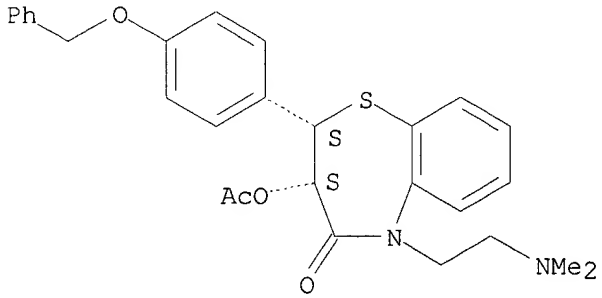
IT **84903-71-9P 84903-72-0P 84903-73-1P**
84903-74-2P 84903-75-3P 84903-76-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 84903-71-9 CAPLUS
CN 1,5-Benzothiazepin-4(5H)-one,
3-(acetyloxy)-5-[2-(dimethylamino)ethyl]-2,3-
dihydro-2-[4-(phenylmethoxy)phenyl]-, cis-(+)- (9CI) (CA INDEX NAME)

Rotation (+). Absolute stereochemistry unknown.

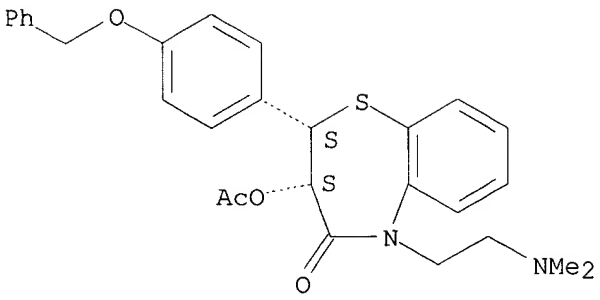


RN 84903-72-0 CAPLUS
CN 1,5-Benzothiazepin-4(5H)-one,
3-(acetyloxy)-5-[2-(dimethylamino)ethyl]-2,3-
dihydro-2-[4-(phenylmethoxy)phenyl]-, monohydrochloride, cis-(+)- (9CI)
(CA INDEX NAME)

Rotation (+). Absolute stereochemistry unknown.



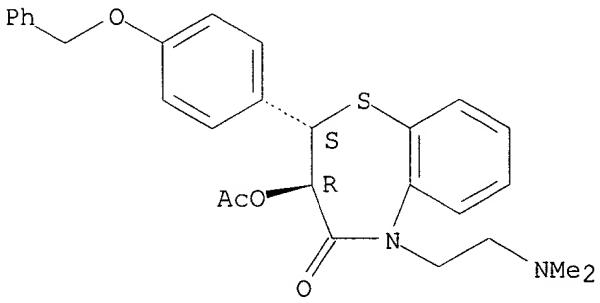
● HCl



● HCl

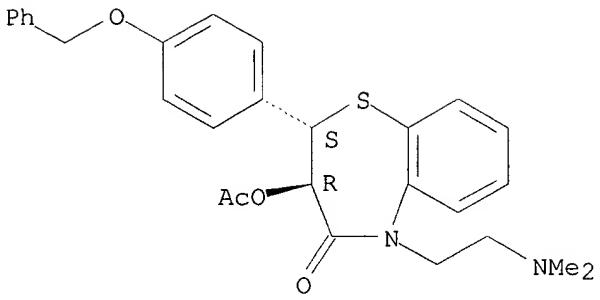
RN 84903-73-1 CAPLUS
CN 1,5-Benzothiazepin-4(5H)-one,
3-(acetyloxy)-5-[2-(dimethylamino)ethyl]-2,3-
dihydro-2-[4-(phenylmethoxy)phenyl]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 84903-74-2 CAPLUS
CN 1,5-Benzothiazepin-4(5H)-one,
3-(acetyloxy)-5-[2-(dimethylamino)ethyl]-2,3-
dihydro-2-[4-(phenylmethoxy)phenyl]-, monohydrochloride, trans- (9CI)
(CA
INDEX NAME)

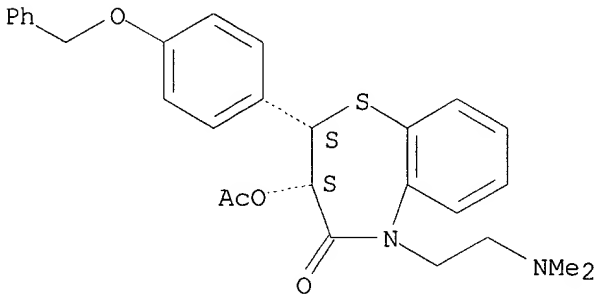
Relative stereochemistry.



● HCl

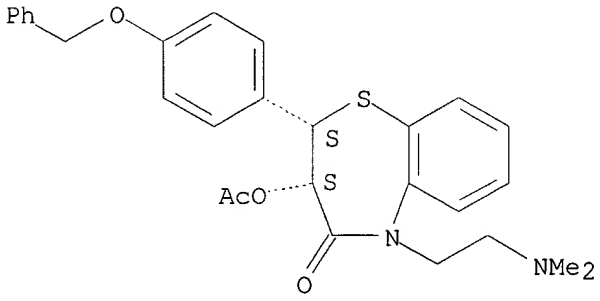
RN 84903-75-3 CAPLUS
CN 1,5-Benzothiazepin-4(5H)-one,
3-(acetyloxy)-5-[2-(dimethylamino)ethyl]-2,3-
dihydro-2-[4-(phenylmethoxy)phenyl]-, cis-(-)- (9CI) (CA INDEX NAME)

Rotation (-). Absolute stereochemistry unknown.



RN 84903-76-4 CAPLUS
CN 1,5-Benzothiazepin-4(5H)-one,
3-(acetyloxy)-5-[2-(dimethylamino)ethyl]-2,3-
dihydro-2-[4-(phenylmethoxy)phenyl]-, cis- (9CI) (CA INDEX NAME)

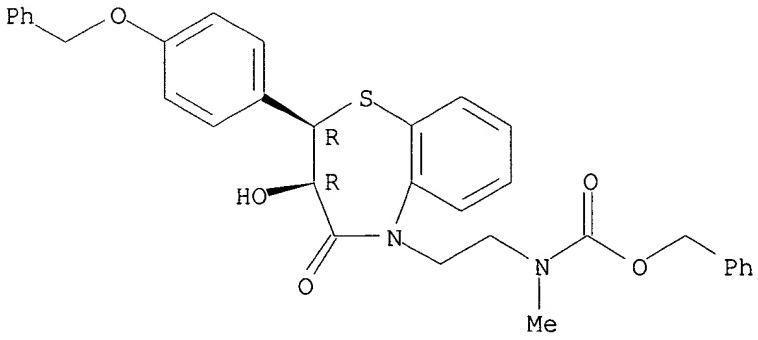
Relative stereochemistry.



L18 ANSWER 11 OF 11 CAPLUS COPYRIGHT 2001 ACS
IT **68767-01-1P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and hydrolysis of)
RN 68767-01-1 CAPLUS
CN Carbamic acid,
[2-[3,4-dihydro-3-hydroxy-4-oxo-2-[4-(phenylmethoxy)phenyl]-
1,5-benzothiazepin-5(2H)-yl]ethyl]methyl-, phenylmethyl ester, cis- (9CI)
(CA INDEX NAME)

Relative stereochemistry.



=> d ti

L18 ANSWER 1 OF 11 CAPLUS COPYRIGHT 2001 ACS
TI Synthesis of the metabolites of clentiazem

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	25.74	394.15

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-1.18

FILE 'REGISTRY' ENTERED AT 11:47:58 ON 06 MAY 2001
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

STRUCTURE FILE UPDATES: 4 MAY 2001 HIGHEST RN 334719-66-3
DICTIONARY FILE UPDATES: 4 MAY 2001 HIGHEST RN 334719-66-3

TSCA INFORMATION NOW CURRENT THROUGH January 11, 2001

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

Structure search limits have been increased. See HELP SLIMIT
for details.

=> s clentiazem
L19 3 CLENTIAZEM

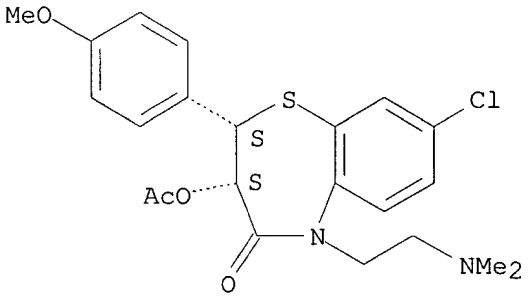
=> d

L19 ANSWER 1 OF 3 REGISTRY COPYRIGHT 2001 ACS
RN 96128-92-6 REGISTRY
CN 1,5-Benzothiazepin-4(5H)-one, 3-(acetyloxy)-8-chloro-5-[2-(dimethylamino)ethyl]-2,3-dihydro-2-(4-methoxyphenyl)-, (2S,3S)-, (2Z)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 1,5-Benzothiazepin-4(5H)-one, 3-(acetyloxy)-8-chloro-5-[2-(dimethylamino)ethyl]-2,3-dihydro-2-(4-methoxyphenyl)-, (2S-cis)-, (Z)-2-butenedioate (1:1)
OTHER NAMES:
CN **(S,S)-Clentiazem maleate**
CN **Clentiazem maleate**
CN TA 3090
FS STEREOSEARCH
MF C22 H25 Cl N2 O4 S . C4 H4 O4
CI COM
LC STN Files: BEILSTEIN*, BIOBUSINESS, BIOSIS, BIOTECHNO, CA, CAPLUS, CASREACT, CBNB, DDFU, DRUGPAT, DRUGU, DRUGUPDATES, EMBASE, IPA, MRCK*, PHAR, PROMT, RTECS*, SYNTHLINE, TOXLINE, TOXLIT, USAN, USPATFULL
(*File contains numerically searchable property data)

CM 1

CRN 96125-53-0
CMF C22 H25 Cl N2 O4 S

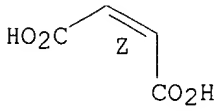
Absolute stereochemistry.



CM 2

CRN 110-16-7
CMF C4 H4 O4

Double bond geometry as shown.



48 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
48 REFERENCES IN FILE CAPLUS (1967 TO DATE)

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=> d his

     (FILE 'HOME' ENTERED AT 11:19:30 ON 06 MAY 2001)

     FILE 'REGISTRY' ENTERED AT 11:19:42 ON 06 MAY 2001
L1              STRUCTURE UPLOADED
L2           50 S L1
L3              STRUCTURE UPLOADED
L4           50 S L3
L5              STRUCTURE UPLOADED
L6           35 S L5
L7          428 S L5 FULL

     FILE 'CAPLUS, USPATFULL' ENTERED AT 11:23:09 ON 06 MAY 2001
L8          452 S L7
L9           10 S L8 AND ((CA OR CALCIUM) (P) CHANNEL)
L10          10 DUP REM L9 (0 DUPLICATES REMOVED)

     FILE 'REGISTRY' ENTERED AT 11:28:55 ON 06 MAY 2001
L11           2 S MIBEFRADIL
L12          87 S L8 AND ?BIS

     FILE 'CAPLUS, USPATFULL' ENTERED AT 11:36:48 ON 06 MAY 2001
L13          98 S L8 AND BIS?
L14           4 S L8 AND DIMER

     FILE 'STNGUIDE' ENTERED AT 11:41:50 ON 06 MAY 2001

     FILE 'REGISTRY' ENTERED AT 11:45:18 ON 06 MAY 2001
L15             STRUCTURE UPLOADED
L16           3 S L15
L17          31 S L15 FULL

     FILE 'CAPLUS, USPATFULL, MEDLINE' ENTERED AT 11:46:19 ON 06 MAY 2001
L18          11 S L17

     FILE 'REGISTRY' ENTERED AT 11:47:58 ON 06 MAY 2001
L19           3 S CLENTIAZEM

=> d l18 ti 2-
YOU HAVE REQUESTED DATA FROM FILE 'CAPLUS' - CONTINUE? (Y)/N:y


YOU HAVE REQUESTED DATA FROM 10 ANSWERS - CONTINUE? Y/(N):y

L18  ANSWER 2 OF 11  CAPLUS  COPYRIGHT 2001 ACS
TI   Synthesis, characterization, and Ca2+ antagonistic activity of diltiazem
     metabolites

L18  ANSWER 3 OF 11  CAPLUS  COPYRIGHT 2001 ACS
TI   Metabolism of diltiazem.  I.  Structures of new acidic and basic
     metabolites in rat, dog and man

L18  ANSWER 4 OF 11  CAPLUS  COPYRIGHT 2001 ACS
TI   Preparation of 8-chloro-2,3-dihydro-3-hydroxy-2-(4-alkoxyphenyl)-5-[2-
     (methylamino)ethyl]-1,5-benzothiazepin-4(5H)-ones as cardiovascular
agents
```

L18 ANSWER 5 OF 11 CAPLUS COPYRIGHT 2001 ACS
TI Benzothiazepine derivatives

L18 ANSWER 6 OF 11 CAPLUS COPYRIGHT 2001 ACS
TI 2-(4-Benzyloxyphenyl)-3-acetoxy-5-(2-dimethylaminoethyl)-2,3-dihydro-1,5-benzothiazepin-4-(5H)-ones

L18 ANSWER 7 OF 11 CAPLUS COPYRIGHT 2001 ACS
TI Benzothiazepine derivatives

L18 ANSWER 8 OF 11 CAPLUS COPYRIGHT 2001 ACS
TI 3-Acetoxy-2-(p-alkoxyphenyl)-5-[2-(dimethylamino)ethyl]-2,3-dihydro-1,5-benzothiazepin-4(5H)-one derivs.

L18 ANSWER 9 OF 11 CAPLUS COPYRIGHT 2001 ACS
TI 3-Acetoxy-5-[2-(dimethylamino)ethyl]-2-(p-hydroxyphenyl)-2,3-dihydro-1,5-benzothiazepin-4(5h)-one derivs.

L18 ANSWER 10 OF 11 CAPLUS COPYRIGHT 2001 ACS
TI 3-Acetoxy-2-[4-(benzyloxy)phenyl]-5-[2-(dimethylamino)ethyl]-2,3-dihydro-1,5-benzothiazepin-4(5H)-one derivs.

L18 ANSWER 11 OF 11 CAPLUS COPYRIGHT 2001 ACS
TI Synthesis of the metabolites and related compounds of diltiazem

=> file reg ;s diltiazem

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.31	403.13

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-1.18

FILE 'REGISTRY' ENTERED AT 11:49:12 ON 06 MAY 2001
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

STRUCTURE FILE UPDATES: 4 MAY 2001 HIGHEST RN 334719-66-3
DICTIONARY FILE UPDATES: 4 MAY 2001 HIGHEST RN 334719-66-3

TSCA INFORMATION NOW CURRENT THROUGH January 11, 2001

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Structure search limits have been increased. See HELP SLIMIT for details.

L20 21 DILTIAZEM

=> d

L20 ANSWER 1 OF 21 REGISTRY COPYRIGHT 2001 ACS
RN 144604-00-2 REGISTRY
CN Butanedioic acid, hydroxy-, (2S)-, compd. with (2S,3S)-3-(acetyloxy)-5-[2-

(dimethylamino)ethyl]-2,3-dihydro-2-(4-methoxyphenyl)-1,5-benzothiazepin-4(5H)-one (1:1) (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 1,5-Benzothiazepin-4(5H)-one, 3-(acetyloxy)-5-[2-(dimethylamino)ethyl]-2,3-dihydro-2-(4-methoxyphenyl)-, (2S,3S)-, (2S)-hydroxybutanedioate (1:1) (9CI)

OTHER NAMES:

CN **Diltiazem malate**

CN MK 793

FS STEREOSEARCH

MF C22 H26 N2 O4 S . C4 H6 O5

CI COM

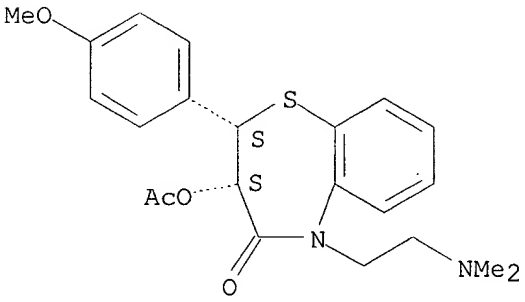
SR US Adopted Names Council

LC STN Files: CA, CAPLUS, DIOGENES, PROMT, TOXLIT, USAN, USPATFULL

CM 1

CRN 42399-41-7
CMF C22 H26 N2 O4 S

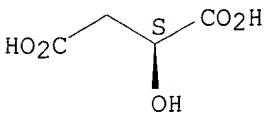
Absolute stereochemistry. Rotation (+).



CM 2

CRN 97-67-6
CMF C4 H6 O5

Absolute stereochemistry.



3 REFERENCES IN FILE CA (1967 TO DATE)
3 REFERENCES IN FILE CAPLUS (1967 TO DATE)

=> d his

(FILE 'HOME' ENTERED AT 11:19:30 ON 06 MAY 2001)

FILE 'REGISTRY' ENTERED AT 11:19:42 ON 06 MAY 2001
L1 STRUCTURE UPLOADED

```
L2            50 S L1
L3               STRUCTURE UPLOADED
L4            50 S L3
L5               STRUCTURE UPLOADED
L6            35 S L5
L7           428 S L5 FULL

     FILE 'CAPLUS, USPATFULL' ENTERED AT 11:23:09 ON 06 MAY 2001
L8           452 S L7
L9            10 S L8 AND ((CA OR CALCIUM) (P) CHANNEL)
L10           10 DUP REM L9 (0 DUPLICATES REMOVED)

     FILE 'REGISTRY' ENTERED AT 11:28:55 ON 06 MAY 2001
L11            2 S MIBEFRADIL
L12           87 S L8 AND ?BIS

     FILE 'CAPLUS, USPATFULL' ENTERED AT 11:36:48 ON 06 MAY 2001
L13           98 S L8 AND BIS?
L14            4 S L8 AND DIMER

     FILE 'STNGUIDE' ENTERED AT 11:41:50 ON 06 MAY 2001

     FILE 'REGISTRY' ENTERED AT 11:45:18 ON 06 MAY 2001
L15              STRUCTURE UPLOADED
L16            3 S L15
L17           31 S L15 FULL

     FILE 'CAPLUS, USPATFULL, MEDLINE' ENTERED AT 11:46:19 ON 06 MAY 2001
L18           11 S L17

     FILE 'REGISTRY' ENTERED AT 11:47:58 ON 06 MAY 2001
L19            3 S CLENTIAZEM

     FILE 'CAPLUS' ENTERED AT 11:48:39 ON 06 MAY 2001

     FILE 'REGISTRY' ENTERED AT 11:48:42 ON 06 MAY 2001

     FILE 'REGISTRY' ENTERED AT 11:49:12 ON 06 MAY 2001
L20           21 S DILTIAZEM

=> d l15
L15 HAS NO ANSWERS
L15              STR
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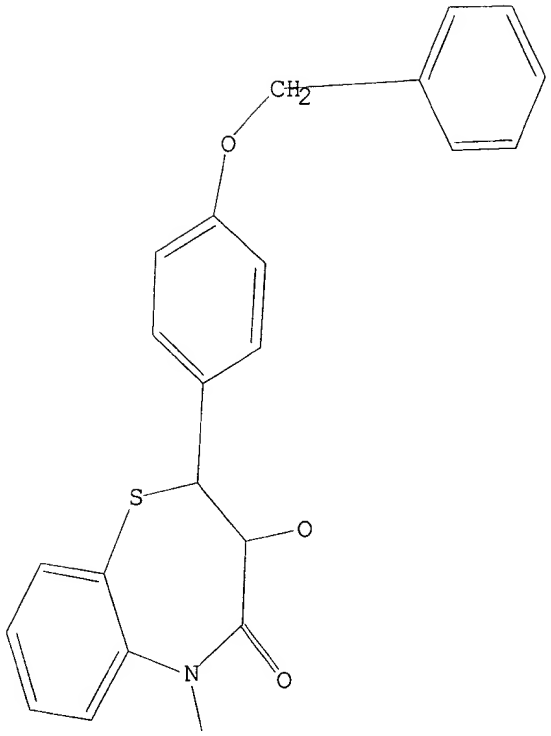
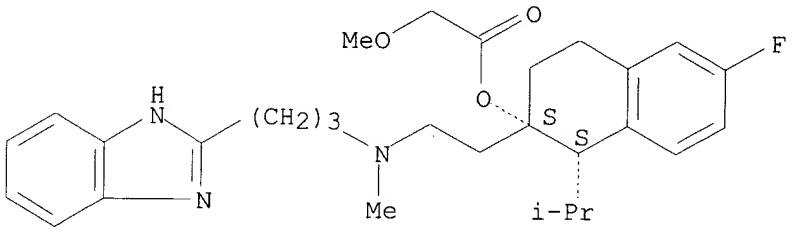


Structure attributes must be viewed using STN Express query preparation.

=>

L11 ANSWER 2 OF 2 REGISTRY COPYRIGHT 2001 ACS
RN 116644-53-2 REGISTRY
CN Acetic acid, methoxy-, (1S,2S)-2-[2-[[3-(1H-benzimidazol-2-yl)propyl]methylamino]ethyl]-6-fluoro-1,2,3,4-tetrahydro-1-(1-methylethyl)-2-naphthalenyl ester (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Acetic acid, methoxy-, 2-[2-[[3-(1H-benzimidazol-2-yl)propyl]methylamino]ethyl]-6-fluoro-1,2,3,4-tetrahydro-1-(1-methylethyl)-2-naphthalenyl ester, (1S-cis)-
OTHER NAMES:
CN (1S,2S)-2-[2-[[3-(1H-Benzimidazol-2-yl)propyl]methylamino]ethyl]-6-fluoro-1-isopropyl-1,2,3,4-tetrahydronaphthalen-2-yl methoxyacetate
CN (1S,2S)-2-[2-[[3-(2-Benzimidazolyl)propyl]methylamino]ethyl]-6-fluoro-1,2,3,4-tetrahydro-1-isopropyl-2-naphthyl methoxyacetate
CN **Mibefradil**
FS STEREOSEARCH
MF C29 H38 F N3 O3
CI COM
SR CA
LC STN Files: ADISINSIGHT, AIDSLINE, BIOBUSINESS, BIOSIS, CA, CANCERLIT, CAPLUS, CASREACT, CIN, DDFU, DIOGENES, DRUGNL, DRUGPAT, DRUGU, DRUGUPDATES, IPA, MEDLINE, MRCK*, PROMT, SYNTHLINE, TOXLINE, TOXLIT, USAN, USPATFULL
(*File contains numerically searchable property data)
Other Sources: WHO

Absolute stereochemistry.



232 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
232 REFERENCES IN FILE CAPLUS (1967 TO DATE)

=>

ACCESSION NUMBER: 1988:549535 CAPLUS
DOCUMENT NUMBER: 109:149535
TITLE: Preparation of [[(heterocyclylalkyl)amino]ethyl]tetrahydronaphthalenes as cardiovascular agents
INVENTOR(S): Branca, Quirico; Jaunin, Roland; Maerki, Hans Peter; Marti, Fraenzi; Ramuz, Henri
PATENT ASSIGNEE(S): Hoffmann-La Roche, F., und Co. A.-G., Switz.
SOURCE: Eur. Pat. Appl., 37 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 268148	A1	19880525	EP 1987-116251	19871104
EP 268148	B1	19911211		
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
DK 8705599	A	19880515	DK 1987-5599	19871026
DK 171349	B1	19960916		
CA 1319144	A1	19930615	CA 1987-550190	19871026
CS 264350	B2	19890712	CS 1987-7874	19871103
AT 70267	E	19911215	AT 1987-116251	19871104
ES 2040234	T3	19931016	ES 1987-116251	19871104
ZA 8708362	A	19880727	ZA 1987-8362	19871106
AU 8780909	A1	19880519	AU 1987-80909	19871109
AU 600769	B2	19900823		
IL 84407	A1	19910916	IL 1987-84407	19871109
JP 63139171	A2	19880610	JP 1987-282287	19871110
JP 2504490	B2	19960605		
US 4808605	A	19890228	US 1987-119114	19871110
HU 60251	A2	19920828	HU 1987-5011	19871111
HU 215915	B	19990329		
FI 8705024	A	19880515	FI 1987-5024	19871113
FI 94414	B	19950531		
FI 94414	C	19950911		
NO 8704757	A	19880516	NO 1987-4757	19871113
NO 172237	B	19930315		
NO 172237	C	19930623		
CN 87107875	A	19880525	CN 1987-107875	19871113
CN 1028991	B	19950621		

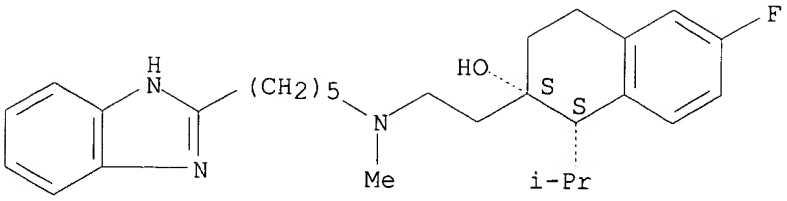
PRIORITY APPLN. INFO.: CH 1986-4565 19861114
EP 1987-116251 19871104

OTHER SOURCE(S): MARPAT 109:149535

IT **116666-64-9P 116666-65-0P 116666-67-2P**
116666-69-4P 116666-73-0P 116666-76-3P
116666-77-4P 116666-78-5P 116666-80-9P
116666-93-4P 116667-02-8P 116667-03-9P
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of, as cardiovascular agent)

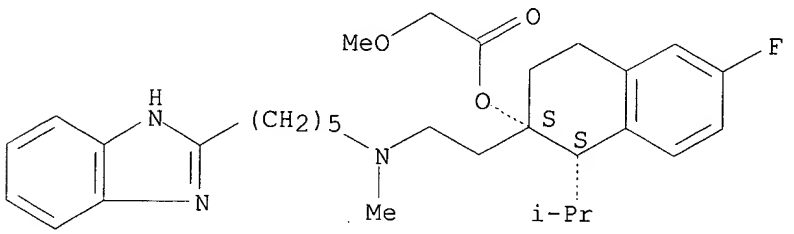
RN 116666-64-9 CAPLUS
CN 2-Naphthalenol, 2-[2-[[5-(1H-benzimidazol-2-yl)pentyl]methylamino]ethyl]-6-fluoro-1,2,3,4-tetrahydro-1-(1-methylethyl)-, (1S-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 116666-65-0 CAPLUS
CN Acetic acid, methoxy-, 2-[2-[[5-(1H-benzimidazol-2-yl)pentyl]methylamino]ethyl]-6-fluoro-1,2,3,4-tetrahydro-1-(1-methylethyl)-2-naphthalenyl ester, dihydrochloride, (1S-cis)- (9CI) (CA INDEX NAME)

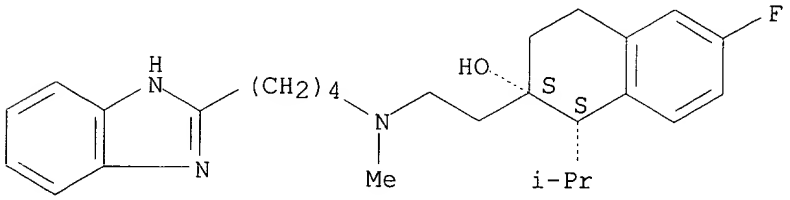
Absolute stereochemistry.



●2 HCl

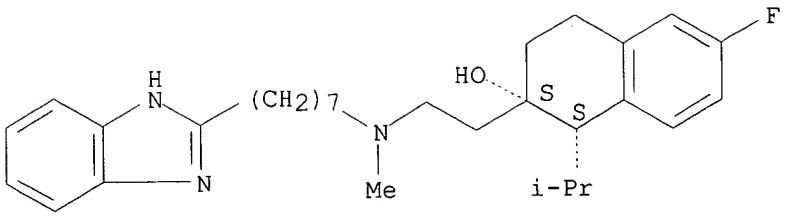
RN 116666-67-2 CAPLUS
CN 2-Naphthalenol, 2-[2-[[4-(1H-benzimidazol-2-yl)butyl]methylamino]ethyl]-6-fluoro-1,2,3,4-tetrahydro-1-(1-methylethyl)-, (1S-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 116666-69-4 CAPLUS
CN 2-Naphthalenol, 2-[2-[[7-(1H-benzimidazol-2-yl)heptyl]methylamino]ethyl]-6-fluoro-1,2,3,4-tetrahydro-1-(1-methylethyl)-, dihydrochloride, (1S-cis)- (9CI) (CA INDEX NAME)

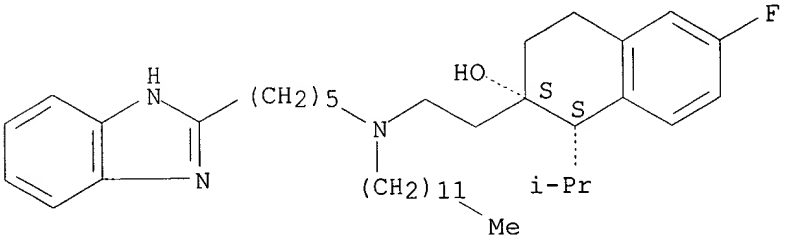
Absolute stereochemistry.



●2 HCl

RN 116666-73-0 CAPLUS
CN 2-Naphthalenol,
2-[2-[[5-(1H-benzimidazol-2-yl)pentyl]dodecylamino]ethyl]-
6-fluoro-1,2,3,4-tetrahydro-1-(1-methylethyl)-, (1S-cis)- (9CI) (CA INDEX
NAME)

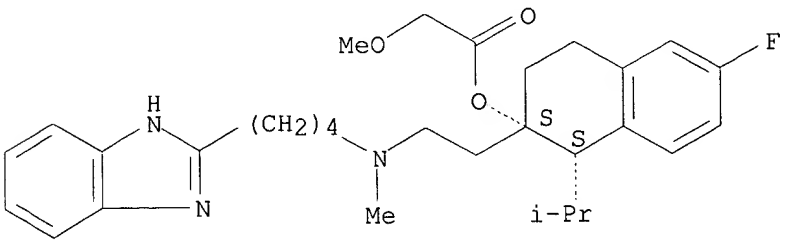
Absolute stereochemistry.



RN 116666-76-3 CAPLUS
CN Acetic acid, methoxy-, 2-[2-[[4-(1H-benzimidazol-2-

yl)butyl]methylamino]ethyl]-6-fluoro-1,2,3,4-tetrahydro-1-(1-methylethyl)-
2-naphthalenyl ester, dihydrochloride, (1S-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



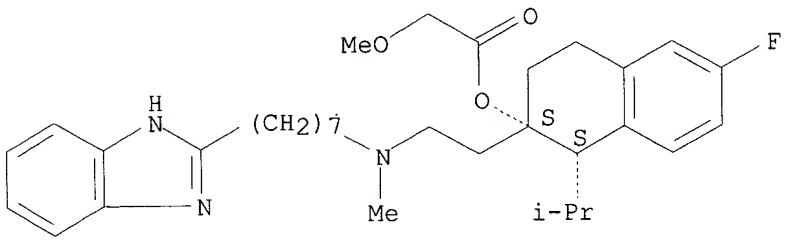
2 HCl

RN 116666-77-4 CAPLUS
CN Acetic acid, methoxy-, 2-[2-[[7-(1H-benzimidazol-2-

yl)heptyl]methylamino]ethyl]-6-fluoro-1,2,3,4-tetrahydro-1-(1-methylethyl)-

2-naphthalenyl ester, dihydrochloride, (1S-cis)- (9CI) (CA INDEX NAME)

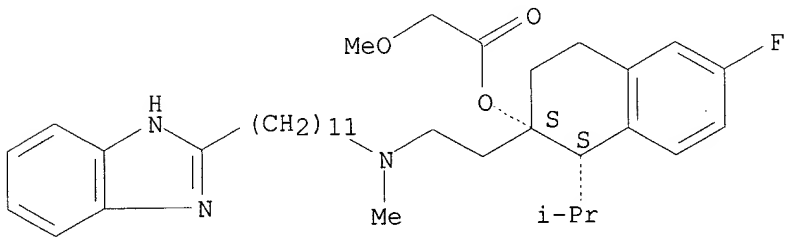
Absolute stereochemistry.



●2 HCl

RN 116666-78-5 CAPLUS
CN Acetic acid, methoxy-, 2-[2-[[11-(1H-benzimidazol-2-yl)undecyl]methylamino]ethyl]-6-fluoro-1,2,3,4-tetrahydro-1-(1-methylethyl)-2-naphthalenyl ester, dihydrochloride, (1S-cis)- (9CI) (CA INDEX NAME)

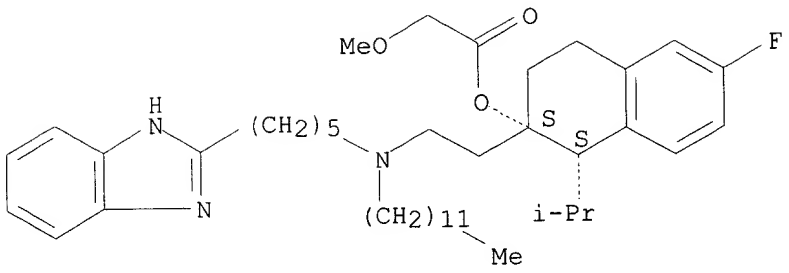
Absolute stereochemistry.



●2 HCl

RN 116666-80-9 CAPLUS
CN Acetic acid, methoxy-, 2-[2-[[5-(1H-benzimidazol-2-yl)pentyl]dodecylamino]ethyl]-6-fluoro-1,2,3,4-tetrahydro-1-(1-methylethyl)-2-naphthalenyl ester, dihydrochloride, (1S-cis)- (9CI) (CA INDEX NAME)

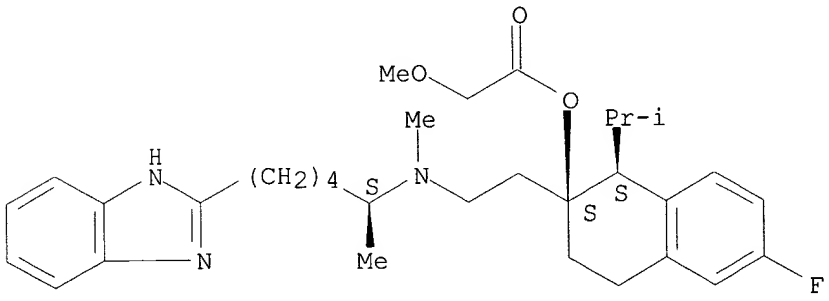
Absolute stereochemistry.



● 2 HCl

RN 116666-93-4 CAPLUS
CN Acetic acid, methoxy-, 2-[2-[[5-(1H-benzimidazol-2-yl)-1-methylpentyl]methylamino]ethyl]-6-fluoro-1,2,3,4-tetrahydro-1-(1-methylethyl)-2-naphthalenyl ester, dihydrochloride, [1S-[1.alpha.,2.alpha.,2(R*)]]- (9CI) (CA INDEX NAME)

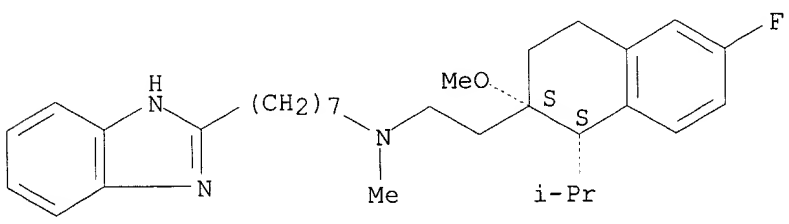
Absolute stereochemistry.



● 2 HCl

RN 116667-02-8 CAPLUS
CN 1H-Benzimidazole-2-heptanamine, N-[2-[6-fluoro-1,2,3,4-tetrahydro-2-methoxy-1-(1-methylethyl)-2-naphthalenyl]ethyl]-N-methyl-, (1S-cis)-(9CI)
(CA INDEX NAME)

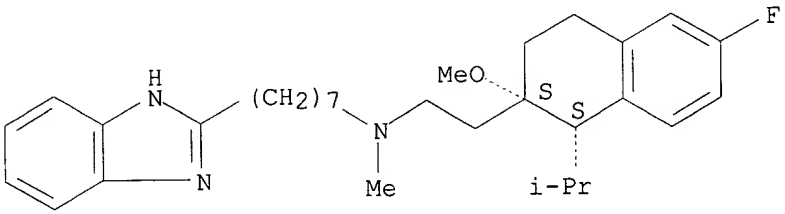
Absolute stereochemistry.



RN 116667-03-9 CAPLUS
CN 1H-Benzimidazole-2-heptanamine, N-[2-[6-fluoro-1,2,3,4-tetrahydro-2-

methoxy-1-(1-methylethyl)-2-naphthalenyl]ethyl]-N-methyl-, dihydrochloride, (1S-cis)- (9CI) (CA INDEX NAME)

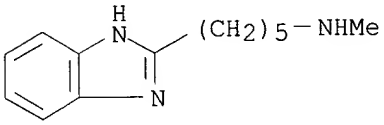
Absolute stereochemistry.



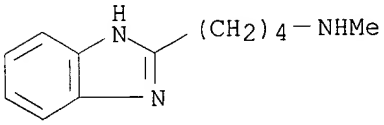
●2 HCl

IT **39650-73-2 116666-66-1 116666-68-3 116666-72-9**
RL: RCT (Reactant)
(reaction of, in prepn. of cardiovascular agents)

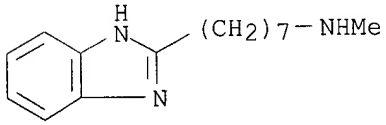
RN 39650-73-2 CAPLUS
CN 1H-Benzimidazole-2-pentanamine, N-methyl- (9CI) (CA INDEX NAME)



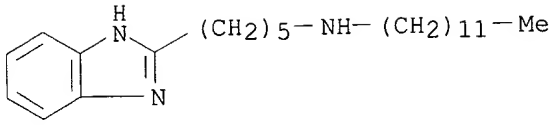
RN 116666-66-1 CAPLUS
CN 1H-Benzimidazole-2-butanamine, N-methyl- (9CI) (CA INDEX NAME)



RN 116666-68-3 CAPLUS
CN 1H-Benzimidazole-2-heptanamine, N-methyl- (9CI) (CA INDEX NAME)



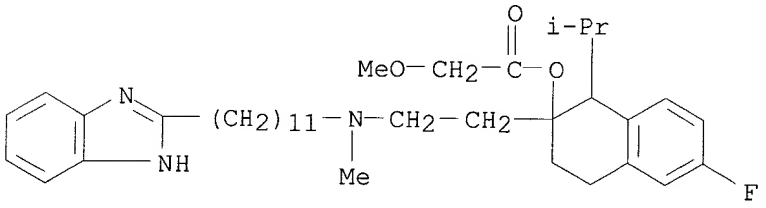
RN 116666-72-9 CAPLUS
CN 1H-Benzimidazole-2-pentanamine, N-dodecyl- (9CI) (CA INDEX NAME)


H
N
N
(CH2)5—NH—(CH2)11—Me

L10 ANSWER 1 OF 10 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 2000:405028 CAPLUS
DOCUMENT NUMBER: 133:217516
TITLE: High affinity interaction of mibefradil with voltage-gated **calcium** and sodium **channels**
AUTHOR(S): Eller, Philipp; Berjukov, Stanislav; Wanner, Siegmund; Huber, Irene; Hering, Steffen; Knaus, Hans-Gunther; Toth, Geza; Kimball, S. David; Striessnig, Jorg
CORPORATE SOURCE: Institut fur Biochemische Pharmakologie, Innsbruck, A-6020, Austria
SOURCE: Br. J. Pharmacol. (2000), 130(3), 669-677
CODEN: BJPCBM; ISSN: 0007-1188
PUBLISHER: Nature Publishing Group
DOCUMENT TYPE: Journal
LANGUAGE: English

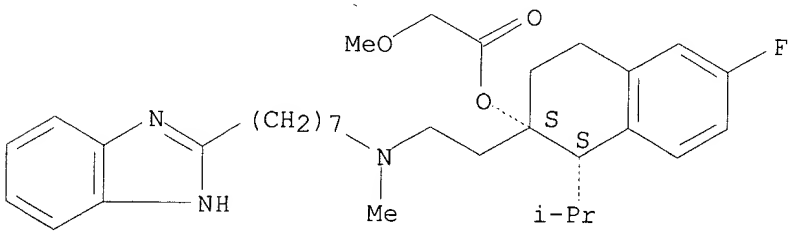
IT **291307-62-5**, Ro 40-6040 **291307-63-6**, Ro 40-6088
RL: BAC (Biological activity or effector, except adverse); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(high affinity interaction of mibeadil with voltage-gated **calcium** and sodium **channels**)

RN 291307-62-5 CAPLUS
CN Acetic acid, methoxy-, 2-[2-[[11-(1H-benzimidazol-2-yl)undecyl]methylamino]ethyl]-6-fluoro-1,2,3,4-tetrahydro-1-(1-methylethyl)-2-naphthalenyl ester (9CI) (CA INDEX NAME)



RN 291307-63-6 CAPLUS
CN Acetic acid, methoxy-, (1S,2S)-2-[2-[[7-(1H-benzimidazol-2-yl)heptyl]methylamino]ethyl]-6-fluoro-1,2,3,4-tetrahydro-1-(1-methylethyl)-2-naphthalenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 46
REFERENCE(S):
(1) Aczel, S; Br J Pharmacol 1998, V125, P447 CAPLUS
(2) Berjukow, S; Br J Pharmacol 1996, V118, P748 CAPLUS
(3) Bezprozvanny, I; Mol Pharmacol 1995, V48, P540

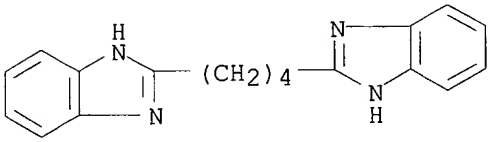
CAPLUS
(4) Birnbaumer, L; Neuron 1994, V13, P505 CAPLUS
(5) Bryson, H; Drugs 1996, V52, P549 CAPLUS
ALL CITATIONS AVAILABLE IN THE RE FORMAT

14 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1995:776400 CAPLUS
DOCUMENT NUMBER: 123:245168
TITLE: Synthesis, Characterization, Spectroscopy, and Magnetism of Dinuclear Azido- and Alkoxo-Bridged Copper(II) Complexes of Bis(2-benzimidazolyl)alkanes. X-ray Structures of [Cu2(tbz)2(CH3O)2](ClO4)2(CH3OH)2, [Cu2(tbz)2(NO3)(CH3O)2](NO3)(CH3OH)2, and [Cu(tbz)(N3)2]2(CH3OH)2 (tbz = Bis(2-benzimidazolyl)propane)
AUTHOR(S): Van Albada, Gerard A.; Lakin, Miles T.; Veldman, Nora; Spek, Anthony L.; Reedijk, Jan
CORPORATE SOURCE: Leiden Institute of Chemistry, Leiden University, Leiden, 2300 RA, Neth.
SOURCE: Inorg. Chem. (1995), 34(19), 4910-17
CODEN: INOCAJ; ISSN: 0020-1669
DOCUMENT TYPE: Journal
LANGUAGE: English

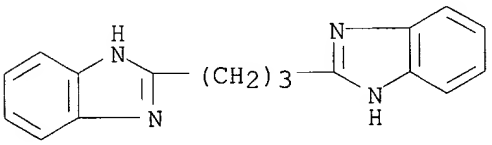
AB A group of new compds. Cu(L)(sol-)(A-)(Hsol), where A = ClO4-, CF3SO3-, BF4-, and NO3-, L = bis(2-benzimidazolyl)propane (abbreviated as tbz) and bis(2-benzimidazolyl)butane (abbreviated as qbz), and Hsol = MeOH and EtOH, and [Cu(tbz)(N3-)(Hsol)] was prepd. and characterized structurally, magnetically, and spectroscopically. Three representative compds. [Cu2(tbz)2(MeO)2](ClO4)2(MeOH)2 (1), [Cu2(tbz)2(NO3)(MeO)2](NO3)(MeOH)2 (5), and [Cu(tbz)(N3)2]2(MeOH)2 (13) were characterized structurally with x-ray diffraction. Crystal data for 1: monoclinic, space group P21/c with a 9.6863(10), b 12.9445(10), c 19.394(2) .ANG., .beta. 113.259(10).degree., and Z = 2. Crystal data for 5: monoclinic, space group P21 with a 9.5497(6), b 12.5073(7), c 17.5920(12) .ANG., .beta. 90.996(6).degree., and Z = 2. Crystal data for 13: orthorhombic, space group Pbca with a 11.3325(7), b 18.7096(16), c 19.2011(16) .ANG., and Z = 4. The structure refinement converged to wR2 = 0.1381, R1 = 0.0534 for 1, wR2 = 0.0674, R1 = 0.0271 for 5, and wR2 = 0.1119, R1 = 0.0701 for 13. The structures 1 and 5 consist of dinuclear units with bridging methoxo groups and one ligand linked to each Cu via the N, providing square planar CuN2O2 chromophores. Structure 5 consists of a dinuclear unit in which one of the Cu atoms is linked to a nitrate O, to yield a unit with two different Cu environments, one square planar and the other square pyramidal. Structure 13 consists also of dinuclear units with the two Cu atoms bridged by .mu.-(1,1)-azido groups. Also each Cu is surrounded by two nitrogens of the ligand and a N of a nonbridging end-on .mu.-(1,1)-azido moiety resulting in a distorted square pyramidal geometry. The Cu-Cu distances (.ANG.) within the dinuclear units are as follows: 1, 2.9827(6); 5, 3.0072(4); 13, 3.2422(9). The Cu-O-Cu bridging angles (deg) are as follows: 1, 102.89(14); 5, 103.97(9), 103.06(9).degree.. The Cu-N-Cu bridging angle for 13 is 104.66(17).degree.. Far-IR spectroscopy shows bands which are characteristic for the bridging Cu2O2N4 chromophore; Cu-O vibrations are found at .apprx.457 and 330 cm-1 for the ethoxo-bridged compds. and at .apprx.390 and 232 cm-1 for the methoxo-bridged compds. The magnetic susceptibility measurements of the alkoxo-bridged compds. display a diamagnetic behavior below room temp. with an estd. exchange parameter 2J of <-600 cm-1. These dinuclear species are EPR silent, and only a weak signal of monomeric impurities is obsd. The .mu.-(1,1)-azido-bridged **dimer** shows a ferromagnetic behavior with a calcd. J value of +23

cm-1 and a weak, very broad isotropic EPR signal at g = 2.14.

IT **4746-56-9**, 1,4-Bis(2-benzimidazolyl)butane
RL: RCT (Reactant)
(for prepn. of copper dinuclear alkoxo-bridged complexes)
RN 4746-56-9 CAPLUS
CN 1H-Benzimidazole, 2,2'-(1,4-butanediyl)bis- (9CI) (CA INDEX NAME)



IT **7147-66-2**, 1,3-Bis(2-benzimidazolyl)propane
RL: RCT (Reactant)
(for prepn. of copper dinuclear azido-, alkoxo- and alkoxo/nitrato-bridged complexes)
RN 7147-66-2 CAPLUS
CN 1H-Benzimidazole, 2,2'-(1,3-propanediyl)bis- (9CI) (CA INDEX NAME)



=>

09/456429
attachment to
Branca et al
reference

L11 ANSWER 2 OF 2 USPATFULL

ACCESSION NUMBER: 89:15067 USPATFULL

TITLE: Tetrahydronaphthalene derivatives as calcium antagonists

INVENTOR(S): **Branca, Quirico**, Basel, Switzerland
Jaunin, Roland, Basel, Switzerland
Maki, Hans P., Basel, Switzerland
Marti, Franzi, Riehen, Switzerland
Ramuz, Henri, Birsfelden, Switzerland

PATENT ASSIGNEE(S): Hoffmann-La Roche Inc., Nutley, NJ, United States (U.S. corporation)

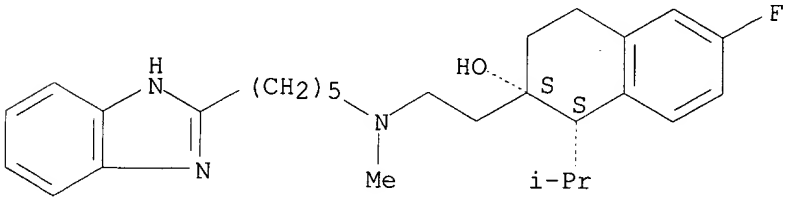
	NUMBER	DATE	
PATENT INFORMATION:	US 4808605	19890228	
APPLICATION INFO.:	US 1987-119114	19871110	(7)

	NUMBER	DATE
PRIORITY INFORMATION:	CH 1986-4565	19861114

DOCUMENT TYPE: Utility
PRIMARY EXAMINER: Schwartz, Richard A.
LEGAL REPRESENTATIVE: Saxe, Jon S.; Leon, Bernard S.; Boxer, Matthew
NUMBER OF CLAIMS: 21
EXEMPLARY CLAIM: 19
LINE COUNT: 2166
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT **116666-64-9P 116666-65-0P 116666-67-2P**
116666-69-4P 116666-73-0P 116666-76-3P
116666-77-4P 116666-78-5P 116666-80-9P
116666-93-4P 116667-02-8P 116667-03-9P
(prepn. of, as cardiovascular agent)

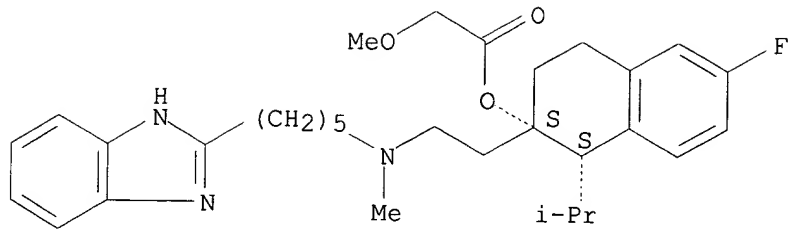
RN 116666-64-9 USPATFULL
CN 2-Naphthalenol, 2-[2-[[5-(1H-benzimidazol-2-yl)pentyl]methylamino]ethyl]-6-fluoro-1,2,3,4-tetrahydro-1-(1-methylethyl)-, (1S-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 116666-65-0 USPATFULL
CN Acetic acid, methoxy-, 2-[2-[[5-(1H-benzimidazol-2-yl)pentyl]methylamino]ethyl]-6-fluoro-1,2,3,4-tetrahydro-1-(1-methylethyl)-2-naphthalenyl ester, dihydrochloride, (1S-cis)- (9CI) (CA INDEX NAME)

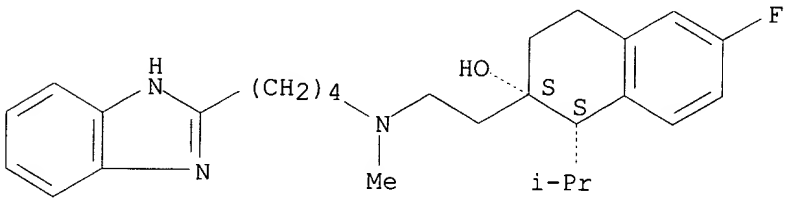
Absolute stereochemistry.



●2 HCl

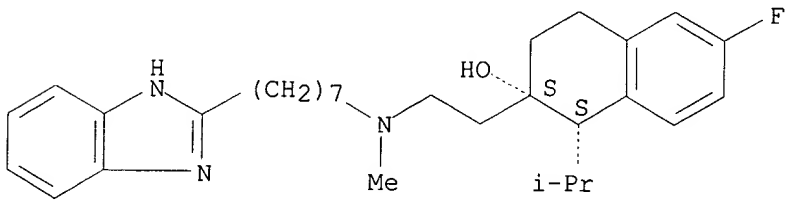
RN 116666-67-2 USPATFULL
CN 2-Naphthalenol,
2-[2-[[4-(1H-benzimidazol-2-yl)butyl]methylamino]ethyl]-6-
fluoro-1,2,3,4-tetrahydro-1-(1-methylethyl)-, (1S-cis)- (9CI) (CA
INDEX
NAME)

Absolute stereochemistry.



RN 116666-69-4 USPATFULL
CN 2-Naphthalenol,
2-[2-[[7-(1H-benzimidazol-2-yl)heptyl]methylamino]ethyl]-6-
fluoro-1,2,3,4-tetrahydro-1-(1-methylethyl)-, dihydrochloride,
(1S-cis)-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.

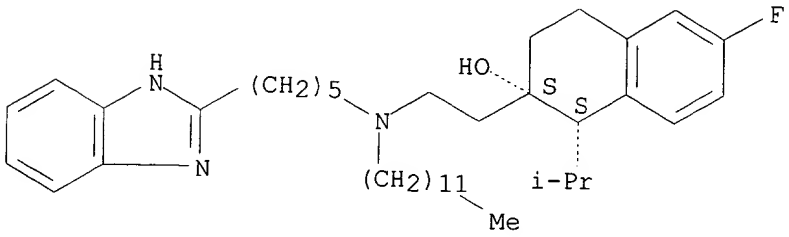


●2 HCl

RN 116666-73-0 USPATFULL
CN 2-Naphthalenol,
2-[2-[[5-(1H-benzimidazol-2-yl)pentyl]dodecylamino]ethyl]-

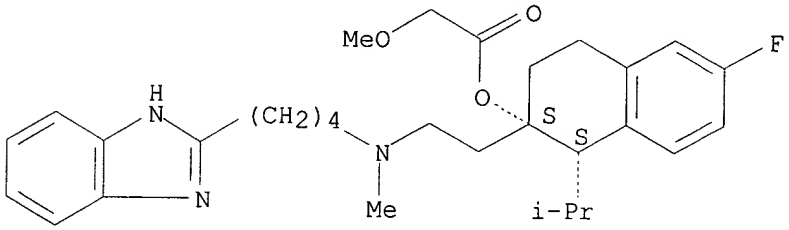
6-fluoro-1,2,3,4-tetrahydro-1-(1-methylethyl)-, (1S-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 116666-76-3 USPATFULL
CN Acetic acid, methoxy-, 2-[2-[[4-(1H-benzimidazol-2-yl)butyl]methylamino]ethyl]-6-fluoro-1,2,3,4-tetrahydro-1-(1-methylethyl)-2-naphthalenyl ester, dihydrochloride, (1S-cis)- (9CI) (CA INDEX NAME)

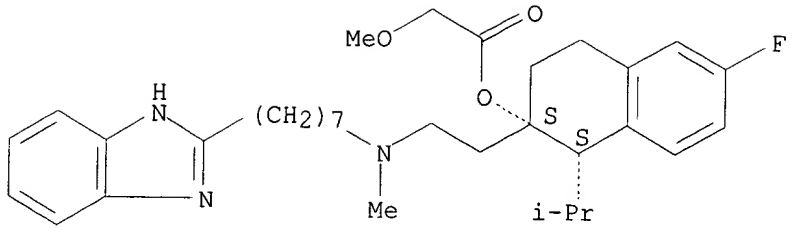
Absolute stereochemistry.



●2 HCl

RN 116666-77-4 USPATFULL
CN Acetic acid, methoxy-, 2-[2-[[7-(1H-benzimidazol-2-yl)heptyl]methylamino]ethyl]-6-fluoro-1,2,3,4-tetrahydro-1-(1-methylethyl)-2-naphthalenyl ester, dihydrochloride, (1S-cis)- (9CI) (CA INDEX NAME)

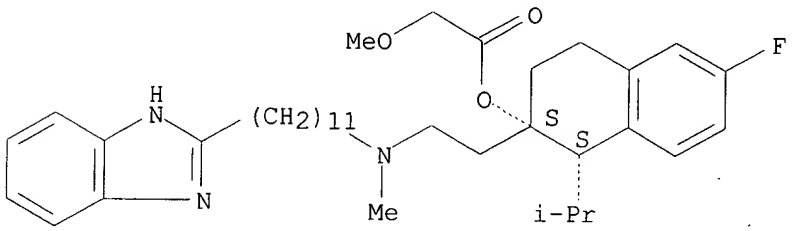
Absolute stereochemistry.



●2 HCl

RN 116666-78-5 USPATFULL
CN Acetic acid, methoxy-, 2-[2-[[11-(1H-benzimidazol-2-yl)undecyl]methylamino]ethyl]-6-fluoro-1,2,3,4-tetrahydro-1-(1-methylethyl)-2-naphthalenyl ester, dihydrochloride, (1S-cis)- (9CI) (CA INDEX NAME)

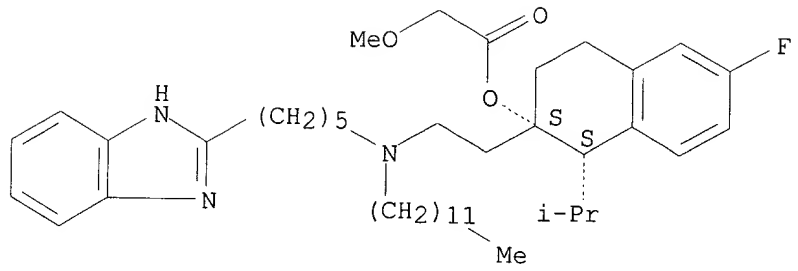
Absolute stereochemistry.



●2 HCl

RN 116666-80-9 USPATFULL
CN Acetic acid, methoxy-, 2-[2-[[5-(1H-benzimidazol-2-yl)pentyl]dodecylamino]ethyl]-6-fluoro-1,2,3,4-tetrahydro-1-(1-methylethyl)-2-naphthalenyl ester, dihydrochloride, (1S-cis)- (9CI) (CA INDEX NAME)

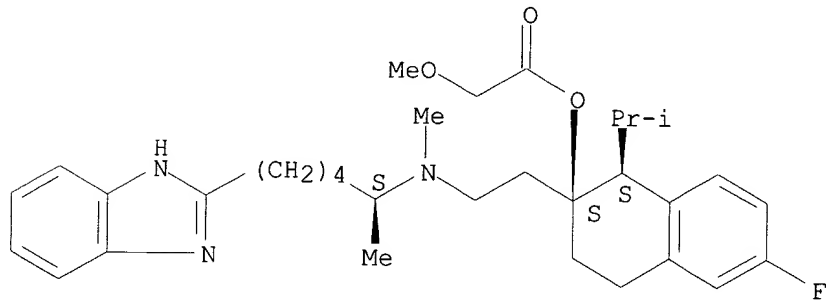
Absolute stereochemistry.



●2 HCl

RN 116666-93-4 USPATFULL
CN Acetic acid, methoxy-, 2-[2-[[5-(1H-benzimidazol-2-yl)-1-methylpentyl]methylamino]ethyl]-6-fluoro-1,2,3,4-tetrahydro-1-(1-methylethyl)-2-naphthalenyl ester, dihydrochloride, [1S-[1.alpha.,2.alpha.,2(R*)]]- (9CI) (CA INDEX NAME)

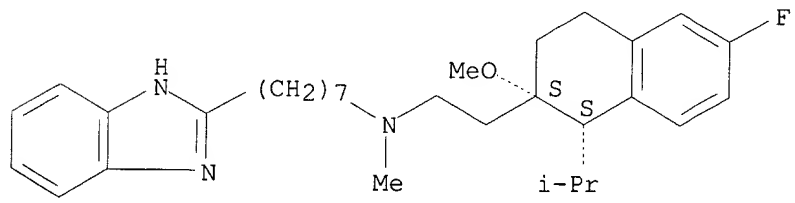
Absolute stereochemistry.



●2 HCl

RN 116667-02-8 USPATFULL
CN 1H-Benzimidazole-2-heptanamine, N-[2-[6-fluoro-1,2,3,4-tetrahydro-2-methoxy-1-(1-methylethyl)-2-naphthalenyl]ethyl]-N-methyl-, (1S-cis)- (9CI) (CA INDEX NAME)

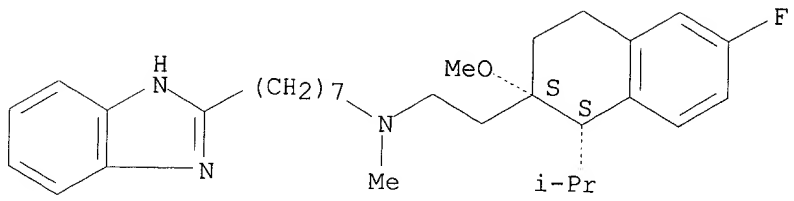
Absolute stereochemistry.



RN 116667-03-9 USPATFULL
CN 1H-Benzimidazole-2-heptanamine, N-[2-[6-fluoro-1,2,3,4-tetrahydro-2-methoxy-1-(1-methylethyl)-2-naphthalenyl]ethyl]-N-methyl-,

dihydrochloride, (1S-cis)- (9CI) (CA INDEX NAME)

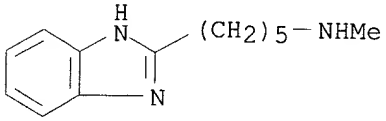
Absolute stereochemistry.



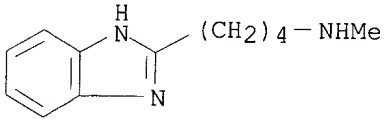
●2 HCl

IT **39650-73-2 116666-66-1 116666-68-3**
116666-72-9
(reaction of, in prepn. of cardiovascular agents)

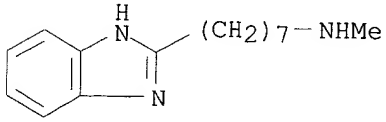
RN 39650-73-2 USPATFULL
CN 1H-Benzimidazole-2-pentanamine, N-methyl- (9CI) (CA INDEX NAME)



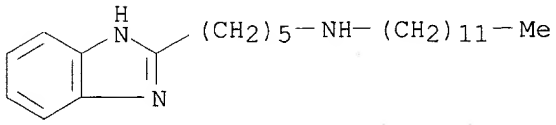
RN 116666-66-1 USPATFULL
CN 1H-Benzimidazole-2-butanamine, N-methyl- (9CI) (CA INDEX NAME)



RN 116666-68-3 USPATFULL
CN 1H-Benzimidazole-2-heptanamine, N-methyl- (9CI) (CA INDEX NAME)



RN 116666-72-9 USPATFULL
CN 1H-Benzimidazole-2-pentanamine, N-dodecyl- (9CI) (CA INDEX NAME)


H
N
N
(CH2)5—NH—(CH2)11—Me

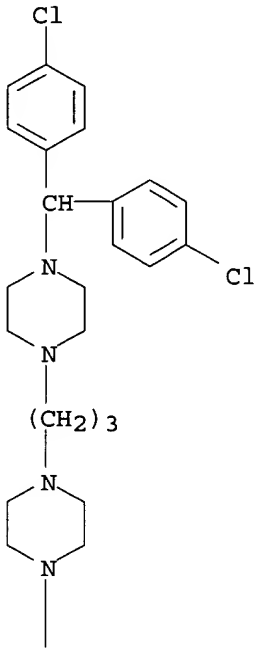
=>

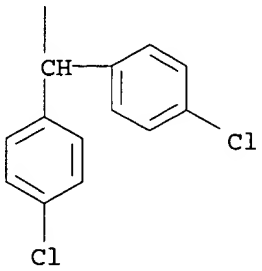
attachment to EP 0122488

RN 94637-59-9 REGISTRY
CN Piperazine, 1,1'-(1,3-propanediyl)bis[4-[bis(4-chlorophenyl)methyl]-, dihydrochloride (9CI) (CA INDEX NAME)
MF C37 H40 Cl4 N4 . 2 Cl H
LC STN Files: CA, CAPLUS

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C6	C6	6	C6	46.150.18	4
C4N2	NC2NC2	6	C4N2	46.383.1	2





●2 HCl

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1

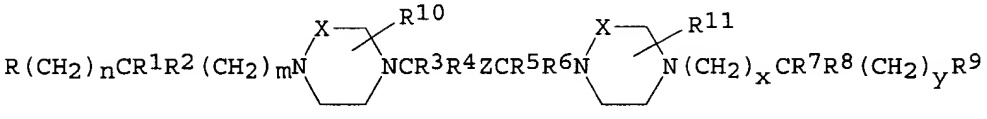
AN 102:78912 CA
TI Bis(piperazinyl- or -homopiperazinyl)alkanes
IN Devlin, John P.; McNeil, Daniel W.; Keirns, James J.; Barsumian, Edward L.
PA Boehringer Ingelheim Ltd., USA
SO Eur. Pat. Appl., 53 pp.
CODEN: EPXXDW
DT Patent
LA German
IC C07D403-06; A61K031-495
CC 28-17 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 63
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 122488	A1	19841024	EP 1984-102979	19840317
	EP 122488	B1	19890607		
	R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
	AT 43843	E	19890615	AT 1984-102979	19840317
	FI 8401081	A	19840922	FI 1984-1081	19840319
	FI 80269	B	19900131		
	FI 80269	C	19900510		
	DK 8401601	A	19840922	DK 1984-1601	19840320
	DK 166022	B	19930301		
	DK 166022	C	19930802		
	NO 8401078	A	19840924	NO 1984-1078	19840320
	NO 162907	B	19891127		
	NO 162907	C	19900307		
	AU 8425891	A1	19840927	AU 1984-25891	19840320
	AU 568122	B2	19871217		
	HU 34016	O	19850128	HU 1984-1102	19840320
	HU 191599	B	19870330		
	DD 219642	A5	19850313	DD 1984-261058	19840320
	ES 530762	A1	19850616	ES 1984-530762	19840320
	ZA 8402037	A	19851224	ZA 1984-2037	19840320
	CA 1218652	A1	19870303	CA 1984-450025	19840320
	PL 141127	B1	19870630	PL 1984-246774	19840320

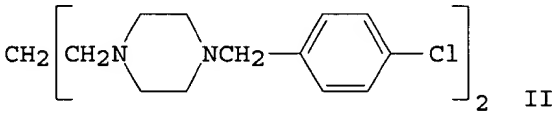
	IL 71291	A1	19871130	IL 1984-71291	19840320
	CS 254971	B2	19880215	CS 1984-1960	19840320
	JP 59176265	A2	19841005	JP 1984-54152	19840321
	ES 535438	A1	19850916	ES 1984-535438	19840827
	ES 535439	A1	19850916	ES 1984-535439	19840827
	ES 535440	A1	19850916	ES 1984-535440	19840827
	SU 1568887	A3	19900530	SU 1986-4027076	19860312
	SU 1574174	A3	19900623	SU 1986-4027087	19860312
	CS 254998	B2	19880215	CS 1986-5529	19860721

PRAI US 1983-477008 19830321
EP 1984-102979 19840317
CS 1984-1960 19840320

GI



I



II

AB The title compds. [I; R,R9 = (un)substituted Ph; R1, R8 = H, alkoxycarbonyl, Me, HOCH2, CO2H, OH, Ph, 4-ClC6H4; R2-R7 = H, Me; R10, R11 = 0-4 Me groups; R1R2, R3R4,R5R6, R7R8 = O; X = CH2, CH2CH2; Z = C1-2 alkylene, hydroxyalkylene; n, m, x, y = 0-3; n + m, x + y .ltoreq. 4] were prepd. Thus, 1-[(4-chlorophenyl)methyl]piperazine was refluxed 17 h in EtOH with Br(CH2)3Cl and the product in Et2O treated with gaseous HCl to give 39% II.4HCl (III). III inhibited mediator release from a rat mast cell prepn. with an IC50 of 3 .mu.M.

ST alkylenebispiperazine prepn antiallergy antiinflammatory; piperazine alkylenebis; alkylation piperazine homopiperazine

IT Inflammation inhibitors and Antiarthritics
(alkylenebis[piperazine] derivs.)

IT Allergy
(inhibitors, alkylenebis[piperazine] derivs.)

IT Alkylation
(of piperazines and homopiperazines)

IT 23145-88-2 40389-65-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(acylation and alkylation of)

IT 1663-67-8 15486-96-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(acylation of (chlorobenzyl)piperazine)

IT 64473-34-3 90876-16-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(alkylation by, of piperazines)

IT 106-55-8 2759-28-6 5321-49-3 17532-19-3 21867-69-6 23145-91-7 23173-57-1 27469-61-0

39577-03-2 41298-98-0 55455-93-1 55513-17-2 69628-75-7
91345-62-9 94637-81-7 94637-82-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(alkylation of)
IT 107-80-2 109-70-6 110-52-1 22286-82-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(alkylation of piperazines by)
IT 110-85-0, reactions 19479-82-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(benzylation of)
IT 352-11-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(benzylation of piperazine by)
IT 75462-56-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(benzylation with, of trimethylene bis[piperazine])
IT 59214-26-5P 70931-28-1P 94637-78-2P 94637-79-3P 94637-80-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);
RACT (Reactant or reagent)
(prepn. and alkylation of)
IT 94637-89-5P 94637-90-8P 94637-91-9P 94637-95-3P 94637-96-4P
94637-97-5P 94637-99-7P
94638-00-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and antiallergy-antiinflammatory activity of)
IT 94637-93-1P 94637-94-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);
RACT (Reactant or reagent)
(prepn. and borohydride redn. of)
IT 94637-98-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and ether cleavage of)
IT 94637-92-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);
RACT (Reactant or reagent)
(prepn. and sapon. of)
IT 94637-31-7P 94637-32-8P 94637-33-9P 94637-34-0P 94637-35-1P
94637-36-2P 94637-37-3P
94637-38-4P 94637-39-5P 94637-40-8P 94637-41-9P 94637-42-0P
94637-43-1P 94637-44-2P
94637-45-3P 94637-46-4P 94637-47-5P 94637-48-6P 94637-49-7P
94637-50-0P 94637-51-1P
94637-52-2P 94637-53-3P 94637-54-4P 94637-55-5P 94637-56-6P
94637-57-7P 94637-58-8P
94637-59-9P 94637-60-2P 94637-61-3P 94637-62-4P 94637-63-5P
94637-64-6P 94637-65-7P
94637-66-8P 94637-67-9P 94637-68-0P 94637-69-1P 94637-70-4P
94637-71-5P 94637-72-6P
94637-73-7P 94637-74-8P 94637-75-9P 94637-76-0P 94644-67-4P
94655-69-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as antiallergy-antiinflammatory agent)
IT 94637-77-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);
RACT (Reactant or reagent)
(prepn., acetylation, and butylation of)